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CAPEC Research Report – 2010
Computer Aided Product-Process Engineering Center

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Preface

This report provides an overview of our research activities and achievements for the period June 2009 to June 2010. An overview of the active research projects is provided in terms of PhD-projects, MSc- & BSc-level exam-projects, post-doctoral and other research projects. A brief overview of the CAPEC software is also included in this report.

An important new development is the increased collaboration between the CAPEC and PROCESS centers with joint projects at different levels (Post-Doc, PhD & MSc). While CAPEC and PROCESS will remain as independent centers, the results from the joint projects will be made available to the member companies of the consortium, to be called in future, the CAPEC-PROCESS consortium.

A number of PhD-projects have been finalized during the period of this report while an equal number of new projects have been started. More specifically, Kavitha C Sataynarayana (PEC09-35), Jamal El Ali Rashed (PEC09-36), Ravendra Singh (PEC09-47) and Ana Carvalho (PEC09-62) have successfully defended their PhD-theses; Merlin Alvarado-Morales (PEC10-13) and Oscar A Prado-Rubio have submitted their PhD-theses; while, Naweed Al-Haque, Klaus R N Hansen, Nor Alafiza Yunus, Alberto Quaglia and Amol S Hukkerikar have started new PhD-projects. Brief descriptions of all currently active PhD-projects can be found in this report. Dr. Ravendra Singh and Dr. Chiara Piccoli have started post-doc positions.

Collaborations with our member companies continues to help us to apply our research results to interesting industrial problems, to get valuable feedback on our methods & tools and to plan our future projects. Collaborations with our friends from academia also help us to develop more comprehensive CAPE/PSE methodologies and techniques. We appreciate these collaborations and we thank our industrial and academic partners for their valuable contributions. During the last 12-months, we have started projects with AstraZeneca, Syngenta, Alfa-Laval, GSK, FMC Corporation, Firmenich and SCG Chemicals from our consortium members, and, Univ of Nancy (France), Chulalongkorn Univ-PPC (Thailand), PROSPECT-UTM (Malaysia), Univ of Kansas (USA) and Auburn Univ (USA) from academia.

We would like to acknowledge the financial support in the form of membership fees from our member companies. For funding of PhD and post-doctoral research projects we would like to thank the Danish funding agencies FTP, NABIT, EFP and ATV and the EU-research programs under FP-6 and FP-7. In addition, we would like to thank the following member companies for their financial support and/or collaboration in research: Alfa Laval Copenhagen, Syngenta, AstraZeneca, Novozymes, and the FMC Corporation. Also, we would like to thank the governments of Malaysia and Mexico for the PhD-scholarships.

Finally, we take this opportunity to thank all co-workers of CAPEC and those from PROCESS who are involved in joint projects for their hard work and dedication. The research results highlighted in this report are their achievements. This is the 13th year since CAPEC was established.

For more information about the CAPEC-PROCESS consortium, please contact Mrs Eva Mikkelsen (eva@kt.dtu.dk).

Rafiqul Gani 1 June 2010

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1. Introduction

Research in CAPEC in collaboration with PROCESS is organized in terms of six research programs (see Fig 1.1). At the inner most level (research programs A, B), the topics are related to fundamental research while at the outer most level (E), the topics are related to applied research. In the intermediate levels (C, D), systematic model-based algorithms, methods and tools are developed by employing the results from the inner levels for use in applied research in the outer level. Since all research programs need numerical tools and databases, research program F supplies this need to all levels. The main theme of the research at CAPEC is to manage the complexity in the systematic analysis and solution of a wide range of product-process engineering problems from various industrial sectors.

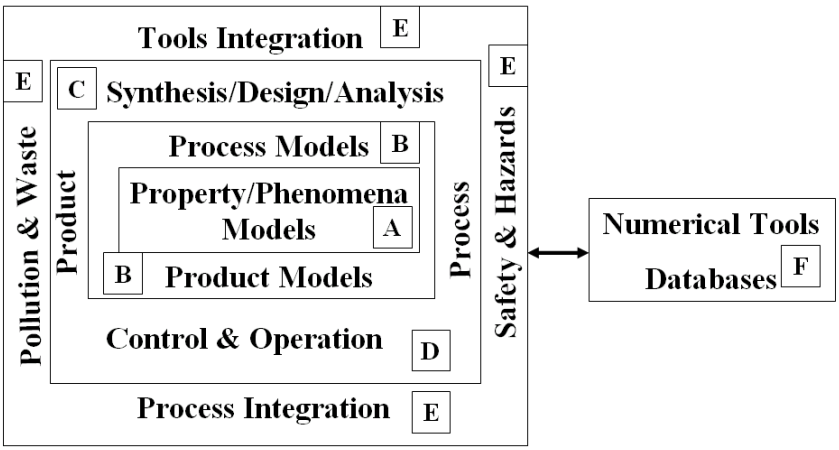


Figure 1.1: Organization of research in CAPEC in terms of research programs

The six research programs are briefly described below:

- *Research Program A – Property and Phenomena Modelling*: deals with theoretical as well as experimental studies of properties (pure component and mixture) of chemical systems and phenomena such as permeability through membranes, reaction kinetics and mass transfer through diffusion. Library of group contribution based models for a wide range of properties of organic chemicals is one of the highlights of program A.
- *Research Program B – Process-Product Modelling and Simulation*: deals with the development of models and model-based simulation systems for prediction of the behaviour and performance of a wide range of chemical and biochemical processes (operating in batch, fed-batch and continuous modes of operation) and a wide range of chemicals based products. A computer-aided modelling system for efficient model development and a collection of process-product models of various types, forms and scales are some of the highlights of program B.
- *Research Program C - Synthesis, Design & Analysis*: deals with development and use of systematic algorithms, methods and tools for synthesis, design and analysis of chemical and biochemical processes and chemicals based products. Techniques such as computer aided molecular and/or mixture design (CAMD), and, process flowsheet design (CAFD) using the reverse approach are some of the highlights of program C.
- *Research Program D - Process Control, Operation & Monitoring*: deals with the development of use of systematic algorithms, methods and tools for process control, operation and monitoring, including process analytical technologies. Techniques for tuning of controller parameters in model predictive control and methods for design of PAT systems are some of the highlights of program D.

- *Research Program E - Process and Tools Integration*: deals with on-line (process) and off-line (tools) integration as well as safety & hazards, sustainability analysis, and integration of process design-control, process-product design and process-process. Integrated software such as ICAS, virtual process-product design lab, SustainPro and their associated methodologies are some of the highlights of program E.
- *Research Program F - Database and Numerical methods*: since CAPEC software needs to be self-sufficient in all respects for use by the industrial consortium companies, CAPEC also maintains a library of numerical methods and databases (properties of chemicals, reaction synthesis, membranes, and analysis equipments). The other research programs benefits from this in terms of data for modelling and improved simulation strategies.

Based on the above, the research objectives of CAPEC can be summarized as:

> *Develop computer-aided systems for efficient and reliable process simulation; for systematic synthesis, design and analysis of sustainable chemical products and their manufacturing processes; for robust control, operation and monitoring of processes from principally chemical, petrochemical, pharmaceutical and biochemical industries. The computer-aided systems are to be developed based on fundamental and/or data-based modelling studies that incorporate correlation and estimation of thermo-physical and phase equilibrium properties as well as modelling the underlying principles / behaviour of the process-product. That is, by managing the complexity in a systematic and efficient manner.*

CAPEC's research is focused (application of a systems approach to problem solution) while the application horizon is wide (oil and gas, petrochemical, chemical and specialty chemical, pharmaceutical, food and bio industrial sectors). CAPEC's strengths can be summarized in terms of its research focus (pioneering work in certain research areas such as modelling; methods for synthesis, design and analysis of process as well as products; process and tools integration), industrial collaboration (dissemination of research results through the industrial consortium as well as collaboration with academia), and contacts (ability to influence developments within chemical engineering and CAPE/PSE). More specifically, CAPEC's contribution in the areas of thermodynamic property modelling, computer-aided molecular-mixture design, targeted reverse approach for product-process design, systematic computer-aided methods and tools for modelling, design, analysis and control are well known within the CAPE/PSE community.

Through CAPEC's large industrial consortium (currently consisting of 30 member companies – see Appendix for a list of member companies), CAPEC co-workers have the unique opportunity to get quick and useful feedback on their developed models, methods and tools as well as insights to the current and future needs of the various industrial sectors represented by the consortium members.

The dissemination of the research results of CAPEC is carried out in terms of:

- *Computational Tools*. Predictive models for reliable property estimation for a wide range of chemicals; generic mathematical models for process operation, product performance; computer-aided tools for product-process synthesis & design, etc., are used by leading industries and close to 50 universities from all over the world.
- *Technology*: Developed systematic methodologies for process-product synthesis, design, analysis and control (& operation), simulation strategies, solvent selection (& design),

pollution prevention, sustainable process-product alternatives, etc., are routinely used to solve industrial problems and in education.

- *Application*: Industrial case studies, tutorial case studies, technology transfer studies and consulting.

1.1 The PROCESS Center

The Center for Process Engineering and Technology is focused on the development of new and innovative processes for industry. PROCESS works at the interface of a number of disciplines, including biotechnology, process engineering and chemistry. The objective is to provide the necessary infrastructure and support to evaluate and implement the next generation of processes in the chemical, bio-based and pharmaceutical sectors in particular. The research is carried out in close collaboration with industry and work is carried out at three levels, namely: laboratory scale experimental process evaluation; model based evaluation of process technology and pilot-scale process validation. Two demonstration units operate in the pilot facilities (one for immobilized enzyme reactions and the other for organic synthesis). Using the results from work at the three levels enables new technology and processes to be evaluated both experimentally and also from the perspective of implementation.

The PROCESS Center is involved in the following large collaborative projects in Denmark and in Europe:

- Bio-petrochemicals is a project established in 2007 with the Danish National Advanced Technology Foundation, DTU Chemistry and Novozymes A/S. It is focused on providing a new route to monomer building blocks from sugars such as glucose to enable an alternative route to chemicals from fossil fuels.
- Sustainable Biodiesel is a project established in 2008 with the Danish National Advanced Technology Foundation, DTU Management, Novozymes A/S, Aarhus University and Emmelev A/S. It is focused on developing a new enzymatic route to biodiesel.
- Towards Robust Fermentation Processes by Targeting Population Heterogeneity at Microscale is a project established in 2009 with the Danish Council for Strategic Research, DTU Systems Biology, DTU Fotonik, Department of Biology (University of Copenhagen), Department of Biotechnology, Chemistry and Environmental Engineering (Aalborg University), Crystal Fibre A/S, Fermenco ApS and Foss A/S. It is focused on characterization and control of the heterogeneity of a population of microorganisms in a fermentation.
- In the pharmaceutical sector several projects sustain the development of the next generation of enzyme based methods for the synthesis of optically pure molecules. The Center is also involved in a 5-year project with Lundbeck aiming at moving from batch towards continuous production, and is a partner in the F3 European consortium established in 2009. The main focus of F3's activities is the development of early stage pharmaceutical leads in collaboration with AstraZeneca Ltd.

The vision of the Center for Process Engineering and Technology is to provide the necessary support to enable the next-generation of processes to be implemented in industry. In this way the new developments in biotechnology, catalysis and separation science alongside process engineering can be translated into industrial practice. New processes with reduced waste, high efficiency and based on all the principles of sustainability can be developed which will help

develop the European industrial sector in the production of chemicals, bio-based materials and chemicals, as well as pharmaceuticals.

1.2 CAPEC-PROCESS Activities

While maintaining their unique center activities, it has been decided to joint forces on a set of research topics of mutual interest within the pharmaceutical, agrochemical and bio & food industrial sectors. The activities shown in Table 1.1 highlight the scope and significance of the research of CAPEC plus the joint activities with PROCESS in terms of the industries where the developed methods and tools are applicable.

Table 1.1: Scope and significance of CAPEC-PROCESS research results shown in terms of industries where they can be applied (1: Includes also oil & gas industries; 2: includes also specialty chemicals; * Solving problems in process modelling, simulation, design, analysis and control)

CAPEC Research Programs	Application of Research Results in terms of Industry					
	Petro-chemicals[1]	Chem-icals[2]	Pharma-ceutical	Agro-chemical	Bio & Food	Aroma
A: Property & Phenomena Modelling						
B: Product & Process Modelling						
C: Synthesis, Design & Analysis						
D: Control, Operation & Monitoring						
E: Process & Tools Integration						
F: Databases & Numerical Methods						

Well developed methods & tools available*	Available methods & tools can easily be adapted if not directly applicable*	Available methods & tools applicable to only a small number of problems*	Needs development*	Work done during 2009-2010
				More focus given in these areas

Some of the challenges for the future are to use our methods and tools to find alternative routes for the production of important chemical products in the petrochemical and chemical sectors using renewable resources; to retrofit or adapt the current processes for changes to bio-based feed materials; to identify new block/platform chemicals, and, to incorporate in all problem solutions the issues related to energy, water, environment and green chemistry.

2. Organization of Activities

The organization of educational and research activities within CAPEC are conducted by CAPEC faculty members together with the researchers and students associated with them, including faculty members and students from PROCESS involved in joint projects. Figure 2.1 highlights these activities, where it can be noted that the research results coming out of the six research programs of CAPEC are disseminated in education and industry.

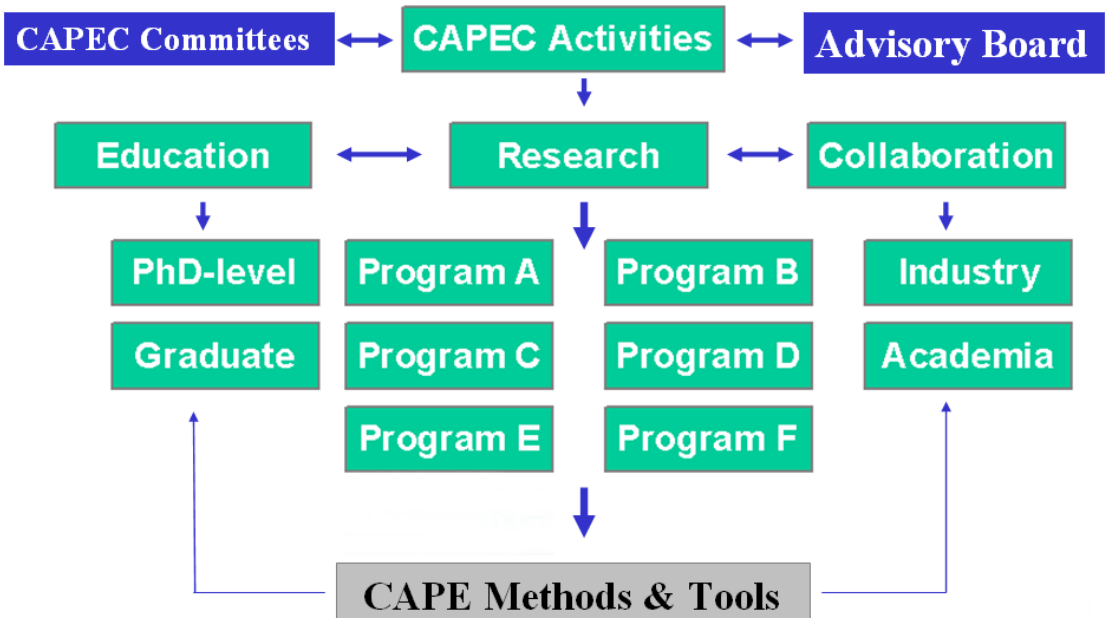
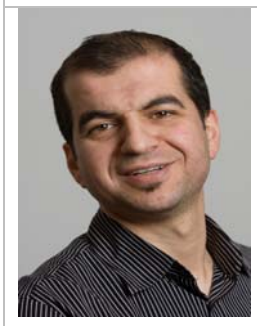


Figure 2.1: Organization of educational and research activities within CAPEC-PROCESS.

2.1 Permanent Members

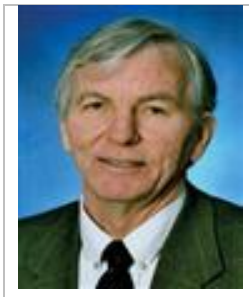
CAPEC	
 **Associate Professor Jens Abildskov (JA)**	Research focuses on development and analysis of correlations and predictive models for thermodynamic properties of fluids for chemical process design. Relationships are sought between molecular structure and thermodynamic properties for simple descriptions of thermodynamic properties. For densities and activities of strongly non-ideal fluids this is offered by statistical mechanical methods based on molecular correlation functions and their connections to fluctuation properties. Examples of applications are: • thermodynamic modeling and microscale simulation for properties relevant to biocatalysis • mixed solvents (liquids and ionic liquids) with dissolved gases, enzymes and pharmaceuticals Exploration is also being made of process energy requirements, to determine the efficiencies of diabatic distillation processes. Reverse engineering is employed in a set of contexts. Collaborations (outside DK) involve researchers in the U.S. and the Netherlands. ***Research Areas:*** *A, B, C, D, F*
 **Reader Karsten Clement (KHC)**	KHC is the Director of BSc Study Program (Chemistry & Chemical Engineering). His research interests lie in process modelling and process control and operation. ***Research areas:*** *B, D*
 **Professor Rafiqul Gani (RaG)**	RaG is Director and Co-founder of CAPEC. His research areas of interest covers modelling (properties, process & product); molecular-mixture (product) design; process synthesis, design & analysis; process-tools integration (PAT, sustainable design, intensification, design-control); and, development of computer-aided systems. Some of the currently active research topics are listed below: • Modelling (chemical products, processes and their operations; performance of products; properties of chemical systems) • Synthesis, design and analysis of chemical products and their sustainable processes (CAMD and CAFD) • Development of methods for sustainable process design; for process intensification; for integration of design-control; for model-based product quality control • Development of integrated computer-aided systems (ICAS, PAT,

	SustainPro, Databases) Applications in petrochemical, chemical, specialty chemical, agrochemical, food and pharmaceutical industries ***Research Areas:*** *A, B, C, D, E, F*
 **Assistant Professor Gürkan Sin (GSI)**	GSI's research covers systematic methods and tools for understanding, design, operation and control of (bio)chemical processes; modeling, control & system identification; uncertainty theory (global uncertainty/sensitivity analysis) & risk assessment; probabilistic-based design paradigm; and, applications in biotechnology, pharmaceutical and water industry. His current research topics of interest are listed below. • Process modelling;model identification • Dynamics & process control; Integrated design & control • Model-based process design; technology configuration; process flowsheet • Uncertainty theory (global uncertainty/sensitivity analysis) & risk assessment • Process design and control under uncertainty; risk-based design Applications in chemical, biochemical (e.g. biotechnology, fermentation technology, etc), pharmaceutical, food and water industries. ***Research areas:*** *B, C, D, E*
PROCESS	
 **Associate Professor Krist V Gernaey (KVG)**	KVG's research covers process modelling; process design/analysis; process control, monitoring & operation; and, process integration-intensification. KVG is a faculty member of the PROCESS center. Currently active research topics are listed below. • Modelling applied to processes (fermentation, biocatalysis, wastewater treatment, food production, pharmaceutical production, biorefineries, ...), using systems of ODEs, population balance models and CFD. • Parameter estimation and model analysis (e.g. sensitivity and uncertainty analysis), i.e. linking process models to plant data • Design of new reactor systems, including microbioreactors for enzymatic reactions and fermentation + systems for continuous production of pharmaceuticals • Design of PAT systems + biorefineries • On-line monitoring of fermentation processes, Process Analytical Technology (pharmaceutical production) Applications in chemical, biochemical (e.g. biotechnology, fermentation technology, etc), pharmaceutical, food and water industries. ***Research Areas:*** *B, C, D, E*

 **Professor John Woodley (JW)**	JW is the head of the PROCESS center and his main research interests lie in the following topics: • Next generation processes (integration of biocatalysis with heterogeneous and homogeneous catalysis; processes based on renewable; green chemistry; pharmaceutical processes; and, biorefineries). • Methodology (process intensification; reactor design; evaluation methodologies) Applications in chemical, biochemical (e.g. biotechnology, fermentation technology, etc), pharmaceutical, food industries. ***Research areas:*** *A, B, C E*
Secretary	
 **Eva Mikkelsen (EVA)**	Eva is the administrative secretary for the CAPEC and PROCESS centers and the CAPEC-PROCESS consortium. Eva also serves as the secretary for the editorial office of the Computers and Chemical Engineering journal office.

2.2 Emeritus

 **Associate Professor Gunnar Jonsson (GJ)**	GJ is an associate member of CAPEC. His research mainly concerns membrane technology (membrane formation and structure; membrane module design; membrane bioreactors; integration of reaction-separation) and transport mechanisms and selectivity; polarization, and fouling phenomena related to the use of membranes. GJ has been involved with many EU- and FTP (funding agency in Denmark) funded projects as well as industrial applications of membrane based technologies. GJ will be retiring in 2010.

 **Professor Sten Bay Jørgensen (SBJ)**	SBJ is a co-founder of CAPEC. He retired from a full-time position in 2009, but continues to contribute to CAPEC's research. SBJ's current research interests include design, modelling & operation of biochemical and chemical products and processes; fixed and moving bed reactors and bioreactors; heat integrated distillation; integrated bioreactor and membrane separation; and, methods and tools for modelling product and process functionality for alarm system design, hazop studies and integration of design and control.

3. Research Projects

3.1 List of current research projects

Research at CAPEC is conducted through research projects at various levels: post-doctoral, PhD, MSc, BSc and visitor-collaboration projects. Table 3.1 provides a list of the currently active projects.

Table 3.1 Currently active research projects at all levels

PhD-Projects (Current)							
No.	**Area**	**Personnel**	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
A-55	B, C	Merlin Alvarado Morales	Process-product synthesis, design and analysis through the group-contribution approach	RaG/JW/ KVG	3-2007	2-2010	DTU
A-56	C, D, E	Mohd. Kamaruddin Bin Abd. Hamid	Integration of modelling, design and control for efficient operation of chemical processes	RaG/GSI	6-2007	5-2010	Malaysia
A-57	A, B, C	Elisa Conte	Innovation in integrated chemical product-process design: Development through a model-based systems approach	RaG/JA	7-2007	6-2010	DTU
A-58	B, C	Oscar Andrés Prado Rubio	Modelling and optimization of integrated bioreactor and membrane separation processes	GJ/SBJ	6-2007	5-2010	BioProduction
A-59	A	Rasmus Wedberg	Simulation of proteins	JA	7-2007	6-2010	BioProduction
A-60	A	Martin Dela Ellegaard	Thermodynamic properties and phase equilibria from fluctuation solution theory	JA	2-2008	1-2011	DTU
A-61	A, B	Linfeng Yuan	Membrane assisted enzyme fractionation	GJ/JW	2-2008	1-2011	Novozymes
A-62	B, D	Noor Asma Fazli Bin Abdul Samad	Control of process operations and monitoring of product qualities through hybrid multi-scale model-based analysis	RaG/GSI/ KVG	1-2009	12-2011	Malaysia
A-63	A, B	Carlos Axel Díaz Tovar	Computer modelling of lipid processing technology	RaG/Bent Sarup	3-2008	2-2011	DTU/Alfa Laval
A-67	C	Alicia Román-Martinez	Design of intensified bioprocesses	RaG/JW	7-2008	6-2011	PROMEP, Mexico
A-70	C	Albert Emili Cervera Padrell	Moving from batch towards continuous organic-chemical pharmaceutical production	KVG/SK/ RaG	8-2008	7-2011	DTU
A-71	B, E	Martina Heitzig	Computer-aided modelling for efficient and innovative product-process engineering	RaG/GSI/ PGL	12-2008	11-2011	DTU
A-72	C, E	Philip Lutze	Green chemistry based innovative process-	JW/RaG/	12-2008	11-2011	DTU

			operation synthesis and design				
A-73	A, C	Azizul Azri Bin Mustaffa	Development and analysis of group-contribution^{plus} models for property prediction of organic chemical systems	RaG/GK	4-2009	3-2012	PROSPECT-UTM (Malayisa)
A-77	B, E	Naweed Al-Haque	Modelling of controlled supply of substrates using solid sorbents in biocatalysis	JW/RaG/PT	11-2009	10-2012	DTU/AMBIOCAS/ CAPEC
A-78	E	Klaus Reinholdt Nyhuus Hansen	New product introduction for the pharmaceutical industry	MG/RaG	9-2009	8-2012	DTU Management
A-79	A, C	Nor Alafiza Yunus	Tailor-made design of chemical products: Bio-fuels and other blended products	RaG/JW/ KVG	6-2010	5-2013	PROSPECT-UTM (Malaysia)
A-80	B, C	Wenjing Fu	Process design of chemo-enzymatic synthetic cascades	JW/RaG/AR	4-2008	3-2011	DTU/PROCESS
A-81	B, C, E	Alberto Quaglia	Model-based integrated product-process design-I	RaG/GSI/ Bent Sarup	6-2010	5-2013	Multimod (CAPEC/Alfa Laval)
A-82	B, C, E	Amol S Hukkerikar	Model-based integrated product-process design-I	RaG/GSI/ Bent Sarup	6-2010	5-2013	Multimod (Alfa Laval)
External PhD-Projects (start-end times indicate their stay at CAPEC)							
No.	**Area**	**Personnel**	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
A-74	B, C	Amnart Janthasurak	Methodology and algorithm for design and synthesis of reactive distillation process	SC/RaG	1-2009	7-2009	Chulalongkorn Univ (Thailand)
A-75	A, C	Claudia Leonor Aguirre Céspedes	Group contribution-based estimation of pure component properties of ionic liquids	LC/RaG	2-2009	7-2009	Univ of Antofagasta (Chile)
A-76	B, C	Sascha Sansonetti	Ethanol production from diary wastes (RCW): Feasibility , optimization & modelling	GSI	9-2009	9-2010	Italy/CAPEC
A-83	C, E	Susilpa Bommareddy	A framework for computer aided process flowsheet design	MRE/RaG	4-2010	7-2010	Auburn Univ (US)/CAPEC
Research Projects (Post-Doc)							
No.	**Area**	**Personnel**	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
B-30	D	Jakob Kjøbsted Huusom	Model identification and optimal tuning for model predictive controllers	JBJ/NKP/ SBJ	12-2008	11-2010	IMM/KT
B-31	B, C, D	Ricardo Morales Rodriquez	Integrated modeling for simulation and design of novel enzymatic processes	GSI/KVG/ AM	6-2009	5-2010	FTP

B-32	B, C	Ravendra Singh	Systematic framework for design and adaption of F3 production processes	Jw/RaG/ KVG	9-2009	2-2011	F3-EU project
B-33	A, B	Chiara Piccoli	Prediction of phase equilibria involving phase transition catalysts	RaG/ P Piccione	4-2010	3-2012	Syngenta
MSc-Projects							
No.	**Area**	**Personnel**	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
C-73	C	Nor Alafiza Yunus	Chemical product design	RaG	5-2009	8-209	UTM, Malaysia
C-74	E	Gregory Guillotin	Sustainable process design: bioethanol production	RaG	6-2009	9-2006	ENSIC, Toulouse
C-75	E	Marie Capron	Hazards and safety analysis	GSI	6-2009	9-2009	ENSIC, Toulouse
C-76	C	Michele Mattei	Computer aided chemical product design	RaG	10-2009	3-2010	30 point
C-?	E	Nutchanat Iyara	Sustainable design for an olefin process	KS/RaG	7-2009	9-2009	PPC,Thailand /CAPEC
C-?	E	Pongsawat Tansutapanich	Sustainable process design for lignocellulosic-based bioethanol using lifecycle assessment technique	PM/RaG	7-2009	9-2009	PPC, Thailand /CAPEC
C-85	D	Dawid Bialas	Model predictive control for reactor-separator recycle system	GSI/JKH/ JBJ	1-2010	6-2010	
C-86	D	Kristoffer Johansen	Control analysis towards multivariate operation of a solvent recovery plant	GSI/SBJ	3-2010	6-2010	
C-87	E	Naruporn Narot	Sustainable process design study of cellulosic-based biofuels	PM/RaG	5-2010	9-2010	PPC, Thailand /CAPEC
C-88	B, C	Preeyaporn Saengwirun	Development of economic analysis methods and tools for process design	KS/RaG	5-2010	9-2010	PPC,Thailand /CAPEC
C-89	C	Jeerawat Wannaborworn	Solvent-based separation	KS/RaG	5-2010	9-2010	PPC,Thailand /CAPEC
C-90	E	Mehboob Nawaz	Optimal biorefinery	RaG/Edwin Zonderwan	6-2010	12-2010	ERASMUS

3.2 CAPEC-PROCESS research programs versus co-workers

Table 3.2 provides an overview of the research programs and the CAPEC-PROCESS personnel involved with them

Research Programs	**CAPEC coworkers & research activities**				
	Faculty[1]	**Post-Docs**[2]	**PhD-students**[2]	**MSc-students**[3]	**Others**[4]
A: Property & Phenomena Modelling	**JA**; (GJ); RaG; KVG; JW	ChP, *ELC*	RAW; (*ELC*); LYF; MEC; ADI; AZM; *NAY*	(*M Mettei*)	*C Aguirre*
B: Product & Process Modelling	**RaG**; JA; (GJ); (SBJ);GSI; KVG; JW	(*RMR*), ChP	(*MAL*); (*ELC*); (*OAP*); LYF; ADI; NAS; ARM; MAT; NAH; WF; *AsH*; AQ	P Saengwirun	*A Janthasurak*; S Sansonetti
C: Synthesis, Design & Analysis	**RaG**; JA; (GJ); (SBJ); GSI; KVG; JW	RS, *ELC*	(*MAL*); (*ELC*) ; MKA; (*OAP*); ADI; ARM; AZM; ACP; PIL; NAH; WF; *NAY*	J Wannaborworn	*A Janthasurak*; S Bommareddy; B C Roughton
D: Control, Operation & Monitoring	**GSI;** (SBJ); KHC; RaG; KVG	JKH	MKA; OAP; NAS	D Bialas; K Johansen	
E: Process & Tools Integration	**RaG**; (GJ), (SBJ); GSI; KVG, JW	RS	MAL; MKA; MAT; PIL; KRNH; *AsH*; AQ	(*N Iyara; P Tansutpanich; M Capron; G Guillotin*); N Narot; M Newaz	(A Carvalho)
F: Databases & Numerical Methods	**JA**; RaG				
Currently active	**5 + 1**	**4**	**15 + *2* + (*3*)**	**6**	**3 + 2**

1: Research area coordinators are indicated in bold; 2: New coworkers who have not yet started are indicated in italic, names in italic-parenthesis indicate coworkers who will soon stop; 3: MSc-students who have finished are indicated by italic-parenthesis; 4: External (or visiting) PhD-students who have returned to their home university are indicated by italic-parenthesis. All other names indicate current coworkers at CAPEC-PROCESS.

3.3 PhD-Research Project Overview

Merlin Alvarado−Morales (MAL)

Supervisors: RaG, KVG, JW
Started: 01-04-2007
Finish: 31-03-2010

Process product synthesis, design, and analysis through the group−contribution approach

The main idea here is to apply the group contribution approach for property estimation to the synthesis, design and analysis of chemical and biochemical processes. Process groups (PGs) are used to represent operations of unit-processes; bonds of PGs are used to represent connecting streams; combination rules for PGs are used to generate process flowsheets; and, PG-contribution based models are used to predict process performances. Using the reverse approach, the designs of the feasible flowsheets are determined. The PG-based flowsheet design concepts developed by d'Anterroches (PEC05-54) has been further extended and verified through the design and analysis of the production of ethanol, succinic acid and diethyl succinate from biomass.

Keywords: *Modelling; process synthesis, design & analysis; process groups; PG-based flowsheet design*

Publications: PEC08-33; PEC09-66; PEC10-13

Albert Emili Cervera Padrell (ACP)

Supervisors: KVG, SK, RaG
Started: 01-08-2008
Finish: 31-07-2011

Moving from batch towards continuous organic-chemical pharmaceutical production

Organic synthesis based pharmaceuticals have traditionally been produced in batch reactors, and it is customary to tailor the synthetic routes to work well in these reactors instead of using reactor set ups designed to handle the relevant chemistry. This results in time-consuming production processes that often need expensive storage of reaction intermediates. As such, batch production also implies that the full benefits of the Process Analytical Technology (PAT) initiative of the FDA cannot be realized in the pharmaceutical production process. In contrast, a continuous production environment may potentially lead to improved safety against, for example, runaway reactions, higher productivity, reduced costs, and reduction or elimination of stocks. The aim of this PhD project is to develop continuous operation units optimized for a certain type of reaction or separation process, ideally preserving flexibility. Such approach should yield a methodology and a set of toolboxes applicable to similar design problems.

Keywords: *Batch-to-continuous; pharmaceutical processes; reactions-reactors; synthesis routes*

Martin D Ellegaard (MEC)

Supervisors: JA
Started: 01-02-2008
Finish: 28-03-2011

Thermodynamic properties and phase equilibria from fluctuation solution theory

Motivation of this project is the accurate solubility estimates and optimal solvent selection that are important for design and analysis of downstream separation processes. In particular, the behaviour of solids in mixed solvents that is difficult to predict as extrapolation of solubility properties between solvents is not straightforward is being investigated. Another objective of this PhD-project is the application of the statistical mechanical fluctuation solution theory to the prediction of gas solubilities in ionic liquids through a group contribution approach.

***Keywords**: Solubility prediction; solvent selection; fluctuation solution theory*

Publications: PEC09-33; PEC10-04; PEC10-05

ELISA CONTE (ELC)

Supervisors: RaG
Started: 15-07-2007
Finish: 14-07-2010

Innovation in integrated chemical product-process design: Development through a model-based systems approach

Development and verification of the methods and tools for the design and analysis of liquid formulated products such as shampoos, paints, sunscreens, hair sprays, etc., are the objectives of this PhD-project. The formulations typically consist of active ingredients (AIs), solvents and additives and need to match specific targets related to product quality, function and performance. The development of systematic methodologies, tools and strategies is necessary in order to efficiently organize the design related activities and improve thereby, the design and evaluation of these chemicals based formulated products. Here, a hybrid concept is adopted, where computer-aided model-based tools perform a fast screening of alternatives to minimize the search space within which the optimal solution is likely to be found. Experiments are then employed for the final testing, verification and selection. This methodology is included in the *Virtual* Product–Process Design Lab software, which performs virtual experiments related to process-product design.

***Keywords:** Property modelling; mixture design; liquid formulated products; virtual product-process design lab*

Publications: PEC09-03; PEC09-72; PEC10-19

Carlos Axel Díaz-Tovar (ADI)

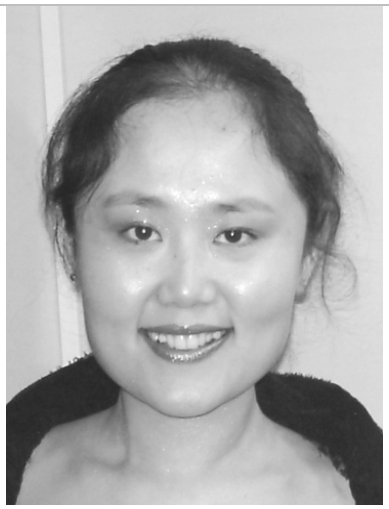
Supervisors: RAG; Bent Sarup (Alfa Laval)
Started: 01-05-2008
Finish: 30-04-2011

Computer aided modelling of lipid processing technology

The production of edible fats and oils, like many other chemical processes, involves a wide range of processing steps, from crude edible oil (vegetable) extraction to the final product. However, unlike the chemical processes, the state of the art in process modelling and simulation has only to a very limited extent penetrated this industry, and part of the reason is the complex nature of the lipid systems involved. Modelling and validation of physical properties of the most representative chemical species and their mixtures occurring in the edible oil industry, as well as optimization of the associated unit operations and process sections are the main objectives of this PhD project. A database of lipid compounds, their important physical properties and models to predict the missing properties have been developed and linked to process simulators to perform simulations for verification and optimization of process design alternatives.

Keywords: *Edible oil industry; lipids; physical properties; process simulation, design & optimization*

Publications: PEC09-65; PEC10-16



Wenjing Fu (WFu)

Supervisors: JW, RaG, AR
Started: 01-04-2008
Finish: 31-03-2011

Process design of chemo-enzymatic synthetic cascades

Limited fossil resources and the unstable oil price make it increasingly important to create new chemical processes based on renewable resources. For many of these new processes a combination of enzymatic as well as heterogeneous and homogeneous catalysis will be required to direct the reaction toward the desired products. In many chemo-enzymatic synthesis processes, even a small reaction pathway, there are many alternative technologies. Thus, there is a need for a systematic methodology capable of evaluating different processes in order to identify the optimal set of products and the best route for producing them. In particular this PhD project will focus on the design of chemo-enzymatic synthetic cascades from glucose to 2,5-furandicarboxylic acid (FDA) as a case study. The process will form the basis of process / cost models for sensitivity analysis and to set targets for catalyst and process improvements.

Keywords: *Process design; chemo-enzymatic synthesis; biorefinery; process-cost models; process evaluation*

Publications: Food & Bioproducts Processing, 88 (2010)

Amol Shivajirao Hukkerikar (ASH)

Supervisors: RaG, GSI,
Bent Sarup (Alfa Laval).
Start: 15-06-2010
Finish: 14-06-2013

Model based integrated product-process design – I

One of the common ways to match the desired product-process characteristics is through trial and error based experiments that can be expensive and time consuming. An alternative approach is the use of a systematic model-based framework replacing some of the time consuming and/or repetitive experimental steps. The main objective of the project is to develop and evaluate model-based tools and methodologies for improving the operation of existing installations for defined products in the edible oil and biofuel industries. Parameters such as operating cost, product yield, emission levels and sustainability metrics will be used to compare alternatives. It is expected that this will be applicable both for optimizing/upgrading and retrofitting of existing process plants as well as for the design of new processing plant. This research work aims to introduce a paradigm shift in product-process design through application of CAPE/PSE tools.

Keywords: *Model-based framework; integrated process-product design, edible oil; biofuel; CAPE/PSE tools*

Mohd. Kamaruddin bin Abd. Hamid (MKA)

Supervisors: RaG, GSI
Started: 01-07-2007
Finish: 30-12-2010

Integration of modelling, design and control for efficient operation of chemical processes

The aim of this project is to develop a new systematic model-based methodology for integrated process design and controller design (*IPDC*) for chemical processes. The *IPDC* problem is formulated as an (optimization) mathematical programming problem, whose solution is decomposed into four sub-problems: (i) pre-analysis; (ii) design analysis; (iii) controller structure design analysis; & (iv) final selection and verification, which are easier to solve in a specified sequence. The methodology manages the complexity through the use of thermodynamic-process insights and the reverse design approach to arrive at the final process design–controller design decisions. The developed methodology has been applied for the design of: a single reactor; a single separator; a reactor–separator-recycle system; and was found to provide effective solutions satisfying the design, control and cost targets. Current work is developing additional case studies as well as integrated model-based software.

Keywords: *Integration of design-control; controller structure; manage complexity; decomposition method*

Publications: PEC09-53; PEC09-66; PEC10-26

Klaus Reinholdt Nyhuus Hansen

Supervisors: Martin Grunow (DTU-management); RaG
Started: 01-09-2010
Finish: 31-08-2010

New product introduction in the pharmaceutical industry

New product introduction process in the pharmaceutical industry deals with identification of important issues associated with developing and testing of new drug products. The overall objective is to increase the speed with which pharmaceutical companies can get their new products into the market, while considering the uncertainty of gaining the approval from regulatory authorities and the high cost of developing a new (drug) product. This requires a careful weighing of the value of increasing sales by fast market introduction against the risk and cost of investments for a fast introduction. The objective of the PhD-project is to develop new tools for assessing the various charted techniques for time-to-market reduction.

Keywords: *Pharmaceutical industry; new drug products; time-to-market; product introduction*

Naweed Al-Haque (NAH)

Supervisors: JW, RaG, Pär Tufvesson.
Started: 15-11-2009
Finish: 14-11-2012

Modelling of controlled supply of substrates using solid sorbents in biocatalysis

With the development of biocatalysts, greener technologies have become more accessible to industry. Biocatalysis has become increasingly common in all industrial sectors such as chemicals, fuels, food and pharmaceuticals. The obvious advantage of this technology is selectivity which is necessary to obtain a high yield of a specific product. The other advantages of operating in benign operating conditions make it an alternative worth investigating. However, in bioprocesses, especially in bioconversions, the substrate and the product may inhibit or damage the biological catalyst or interfere with other components in the reaction medium above a critical concentration. This limitation can be overcome with methods such as slow release of substrates combined with *in-situ* product removal (ISPR) using solid sorbents. This project will focus on the latter issue and in particular for the development of this novel substrate release technique with controlled diffusing rate of the substrate in the reaction medium using a solid resin(s).

Keywords: *Biocatalysis; controlled supply; resins, ISPR; mathematical modelling*

Martina Heitzig (MAT)

Supervisors: RAG, GSI, PGL
Started: 01-12-2008
Finish: 30-11-2011

Computer-aided modelling for efficient and innovative product-process engineering

Computer-aided modelling plays an increasingly important role in various industrial sectors served by chemical and biochemical engineering. Model-based solution approaches are attractive because they are able to provide rapid and reliable screening of process-product alternatives. However, the model generation, testing and validation are time and resource intensive. Also, for a wide range of application of any model-based solution approach, models need to be developed and adapted quickly and reliably. Therefore, there is a need for systematic modelling methods and associated computer-aided tools. The objective of this project is to develop a computer-aided modelling framework together with work-flows for systematic solution of various modelling tasks through a suite of modelling tools that also enable multiscale and multi-dimensional modelling options.

Keywords: *Computer-aided modelling; modelling framework; multiscale; multidimension; ICAS-MoT*

Publications: PEC09-69

Philip Lutze (PIL)

Supervisors: JW, RAG
Started: 01-12-2008
Finish: 30-11-2011

Development of a systematic synthesis/ design methodology incorporating process intensification

The chemical, biochemical and pharmaceutical industry is facing new challenges which need improvements in whole processes. One way to achieve them is through process intensification (PI), which is an engineering strategy to achieve improvements in processing/operation through synthesis/design of the process and/or design of new equipments. The objective of this project is to develop a systematic synthesis/design methodology incorporating PI. The method is based on solid understanding of the underlying principles that promote PI; the generation of alternative designs from a superstructure; the creation of models; the evaluation of the most promising alternatives to identify the best; and finally, the design experiments for verification of the intensified process. Current and future plans include testing and verifying the PI-design methodology through practical case studies from different industrial sectors.

Keywords: *Process intensification; design methodology; process synthesis; superstructure, design of experiments*

Publications: PEC09-64; PEC10-20; PEC10-21

Azizul Azri Mustaffa (AZM)

Supervisors: RaG, GK
Started: 01-04-2009
Finish: 31-03-2012

Development and analysis of GC^{Plus} models for property prediction of organic chemical Systems

Accurate, reliable and efficient prediction of properties is very important in chemical process-product design. However, due to the increased complexity of the molecular structures of chemicals, their wider applications, and demands for greater accuracy, extension and analysis of the current prediction methods as well as development of new models are necessary. Therefore, the combination of group-contribution (GC) and atom connectivity (CI) (the GC^{Plus} approach) that is able to extend the application range of the host property model has been developed and extended to predict the UNIFAC GC-model parameters (see PEC09-17). The objectives of this PhD-project is to analyze the performance of the GC^{Plus} approach in VLE and SLE calculations and based on it, to extend and further develop the GC^{Plus} approach for other versions of the UNIFAC models and to apply the models for chemical process synthesis and design.

Keywords: *GC^{Plus} approach; mixture properties; UNIFAC models; parameter prediction*

Publications: PEC10-18

Oscar Andrés Prado-Rubio (OAP)

Supervisors: GJ, (SBJ)
Started: 01-06-2007
Finish: 31-05-2010

Modeling and optimization of integrated bioreactor and membrane separation processes

The fermentation of Lactic acid by Lactic Acid Bacteria is normally impaired by product inhibition like many other fermentation processes at a certain concentration level of the product or one of the bi-products. Therefore, continuous removal of Lactate from the fermenter will result in a higher productivity and product yield. Integrating separation and fermentation will also enable operation at higher cell densities, thereby providing additional enhanced productivity potential. The objective of this project is to derive, validate and investigate a dynamic model for an integrated bioreactor and electrically driven membrane separation processes. The purpose of this model is to optimize the design and operation of lactic acid fermentation according to different objectives.

Keywords: *Modelling; lactic acid; fermentation; membrane separation; bioreactor*

Publications: PEC09-52; PEC09-59; PEC09-60

Alicia Román Martínez (ARM)

Supervisors: RaG, JW
Started: 01-08-2008
Finish: 31-07-2011

Design of integrated chemo-enzymatic processes

The objective of this project is to develop and apply a flexible framework for design and analysis of integrated chemo-enzymatic processes. The framework consists of a systematic model-based computer aided methodology to identify reliable, feasible and/or improved integrated design options for chemo-enzymatic processes. The framework incorporates tools for process synthesis and optimization, such as, the use of superstructures and strategies for development of mathematical models to find the best route for the synthesis of specified products through an integrated chemo-enzymatic process. The advantages of using this framework is that it permits the saving of valuable experimental resources, which could then be used only for implementation and verification of the design and is able to enumerate and analyze all the possible reaction-separation schemes in the process to locate a reduced search space where the best option could be found. Current work is developing case studies to highlight the application of the framework.

Keywords: *Integrated chemo-enzymatic process; model-based solution; framework for design; optimization*

Publications: PEC09-64

Alberto Quaglia (AQ)

Supervisors: RaG; GSI, Bent Sarup (*Alfa Laval*)
Started: 31-05-2010
Finish: 31-05-2013

Model-based integrated process-product design

Process Simulation is not common in the food and biofuels industries, mainly due to the complexity of thermodynamics and transport properties of the species involved. This project aims to introduce a paradigm shift in product-process design through the application of CAPE/PSE tools in these industries. The research will focus on the use of validated models in the early stages of product-process design in order to eliminate redundant alternative process routes. The objective will be to identify the most promising process route so that the more time consuming and costly steps (computational as well as experimental) can be reduced. To achieve this objective, a systematic framework for computer-aided flowsheet design (CAFD) will be developed and evaluated in collaboration with Alfa Laval. A particular emphasize will be given to deal with uncertainties in data and models.

Keywords: *Model-based solution; process simulation; edible oil & biofuel industries; design under uncertainties*

Noor Asma Fazli Bin Abdul Samad (NAS)

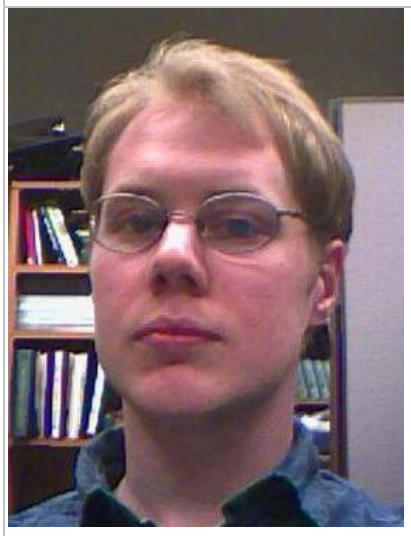
Supervisors: RAG, KVG, GSI
Started: 15-01-2009
Finish: 31-12-2011

Control of process operations and monitoring of product qualities through hybrid multi-scale model-based analysis

The aims of this work are to develop a generic multidimensional model-based framework for batch cooling crystallization processes that can provide a better understanding of crystallization operations and from which it should be possible to generate specific models for simulation and evaluation of different batch cooling crystallization operational scenarios. The framework should the study of crystallization processes in single or multi-dimensional schemes and for a wide range of chemical systems. The generic model should include constitutive models accounting for saturation; primary and secondary nucleations; crystal growth; agglomeration and breakages phenomena. The current version of the developed generic model can handle 1-2 dimensions and the various phenomena occurring during various crystallization operational scenarios. The model and the framework are currently being tested and verified through problems reported in the open literature and applications in process control, product monitoring and optimization.

Keywords: *Modelling framework, generic model; crystallization; process control; product monitoring*

Publications: PEC09-73



Rasmus Wedberg (RAW)

Supervisors: JA, GHP
Started: 01-11-2007
Finish: 31-10-2010

Simulation of Proteins

In this project, molecular modelling and simulation is applied to study solvent effects on lipase B from *Candida Antarctica*, a catalyst commonly applied for a large number of reactions, *e.g.* transesterifications. The enzyme, representative substrates and activated complexes will be simulated in various solvents using molecular dynamics simulations and possibly also QM/MM methods. A number of calculations of properties that can be correlated with the activity, for example, free energy differences and conformational flexibility near the active site, will be carried out. The aim is to make qualitative statements about the effects the solvent will have on the activity. The results will be verified by kinetics measurements performed by our collaborators.

Keywords: *Molecular modelling; molecular dynamic simulation; proteins; solvents; solvent effects*

Publications: PEC09-54

Linfeng Yuan (LFY)

Supervisors: GJ, JW
Started: 15-03-2009
Finish: 01-04-2011

Membrane assisted enzyme fractionation

The aim of this project is to develop a suitable membrane fractionation process and to assess the economics of such membrane processes for industrial scale production for relevant applications such as pharmaceutical and dairy enzyme production. If an efficient process is developed then pilot up-scaling of the membrane fractionation process will be considered. The feasible membrane fractionation process to be considered or investigated will potentially include:

- Electro-membrane filtration
- Charged membranes
- Membrane systems using high frequency pulsation and / or vibration

Feed solution properties such as pH, ionic strength, additives can be chosen as appropriate.

Keywords: *Enzyme fractionation; charged membranes; electro-membrane filtration; industrial scale production*

Nor Alafiza Yunus (NAY)

Supervisors: RAG, JW, KVG
Started: 01-06-2010
Finish: 01-05-2013

Tailor-made design of chemical products: Bio-fuel and other blended products

Product blending is a common activity in the process industry. A naphtha blend for an ethylene plant, for instance, needs to have the right aromatic and paraffinic compositions while the contents of poisoning elements remain below their acceptable limits to protect catalysts. This shows the importance of using the right composition in the blending process as well as fuel blending case. Typically, trial and error experimental methods are used to identify the suitable fuel blend compositions. However, this method can become costly, time-consuming and there is no guarantee that an acceptable product will be found. An appropriate computer aided technique on the other hand, could be very efficient and very likely to identify the optimal chemical blends because they are by nature, time and resource efficient and able to search a wide range of options. The aim of this project is to develop a general blend design methodology for the blending process involving bio-products and petrochemical products and producing a tailor-made fuel-blend.

Keywords: *Tailor-made bio-fuel blends; blend design methodology; bio- and pharmaceutical products*

3.4 External PhD-students (projects)

3.4.1 PhD-students currently visiting CAPEC

Sascha Sansonetti (SSA)

Supervisor: GSI
Started: 01-09-2009
Finish: 30-09-2010

Feasibility, optimization and modelling of ethanol production from dairy wastes

Dairy industry produces a huge amount of wastes which consist of several kinds of the same by-product called "cheese whey". The lactose content in this waste suggests the possibility to produce ethanol by anaerobic fermentation. However, to this day, not enough efforts have been done to ensure a better understanding of the involved mechanisms, thus resulting in a very limited application on an industrial level. This project, after a preliminary 2-year phase in which both process feasibility and optimization have been achieved, is aimed to build a model based on the metabolic pathways involved in the fermentation reaction. The resulting "biochemically structured model" could be useful to give a better understanding of the process and to predict the system behaviour. Eventually, after having tested the model with continuous run data, the project should be concluded with a process sustainability analysis. See also PEC10-09.

Keywords: *Dairy industry; cheese whey; anaerobic fermentation; ethanol production; sustainability analysis*

Susilpa Bommareddy

Supervisors: Mario R Eden (Auburn University, USA); RaG
Started: 21-04-2010
Finish: 18-07-2010

Computer-aided flowsheet synthesis and design using group contribution methods

Process synthesis and design deals with identifying the process flowsheet that includes the required operational tasks, equipments, solvents, etc., and their conditions of operation, quantity, etc., for given input and target process performance. A suitable framework based on the group contribution concept for the above tasks is to be developed. Based on the framework, a user-friendly software tool is to be developed so that computer aided flowsheet synthesis and design can be performed in the same way as computer aided molecular design. Each unit operation/process is represented by a process group together with their connection rules and a flowsheet property model (see PEC05-54) to predict a value indicative of the flowsheet performance. Reverse simulation of each unit operation/process gives their conditions of operation and process design parameters.

Keywords: *Computer-aided flowsheet design; group-contribution concept; process groups; reverse simulation*

3.4.2 Computer aided design of ionic liquids (Claudia Leonor Aguirre Cespedes, University of Antofagasta, Chile) – continuing collaboration

The objectives of this PhD-project is to create a database with all ionic liquids that can be formed through the available groups, predict the properties of these ILs, and extend the group parameter tables to predict properties of those ionic liquids that could not be handled because of the missing group parameters. Due to the large number of potential ionic liquids that can be already formed, it is expected that this database can be used to identify and select ionic liquids with desired (target) properties, as well as to find new properties to be modelled that will be necessary for a wider range of applications of ionic liquids. In this way, the created database of existing and new ILs will be equipped with a search engine to quickly identify the needed IL, if it exists. A database has been created with known and generated ILs; property estimation methods have been collected and tested; a search engine for selection of ILs based on target properties has been developed (PEC10-17).

3.4.3 Methodology and algorithm for design and synthesis of reactive distillation columns (Amnart Janthasurak, Chulalongkorn University – SCG Chemicals, Bangkok, Thailand) – continuing collaboration

The objective of this work is to develop a methodology for design and analysis of reactive distillation columns for multicomponent reactive systems. The concept of driving-force and reverse design approach will be combined to determine near-optimal designs with respect to energy consumption, waste and cost. Hengstebeck's procedure for reduction of multicomponent systems to binary systems will be adapted to "elements" so that multi-element reactive systems can also be reduced to binary element systems. From the binary reactive element driving force and vapor-liquid phase (reactive) diagrams, the already established methods for distillation design will be applied. Here, the driving-force diagram will first be used to identify the location of the maximum driving force (according to the driving force concept, larger driving force implies better separation, less waste, less energy consumption and therefore, lower cost). The reverse approach helps to determine the design of the distillation column that matches the target driving force. Once the reactive distillation design has been obtained, it will be validated with rigorous reactive distillation models and then, if feasible, through experiments. Details of the developed methods and tools can be found in PEC10-01.

3.5 Post-Doctoral Research Project Overview

Jakob K Huusom (JKH)

Supervisors: SBJ (NKP, JBJ)
Started: 01-12-2008
Finish: 31-12-2010

Model identification and optimal tuning for model predictive controllers

In this project we will investigate methods for shortening commissioning times and improving quality in model predictive control applications. The contributions of this project will stem from addressing the problems related to commissioning and maintenance of MPC controllers from several angles. First, the use of process models which are tailored specifically for use with MPC and identification methods that are well suited for use in industrial settings are to be investigated. Second, control performance will be improved through application of several tuning methods to the controller modules. These methods are used for selection of optimal tuning parameters in the controller, estimation of noise statistics and identification of disturbances.

Keywords: *Model predictive control; identification method; control performance; commissioning of MPC*

Publications: PEC09-42; PEC09-58; PEC09-74

Chiara Piccolo (ChP)

Supervisors: RaG, Patrick Piccione (Syngenta)
Started: 01-04-2010
Finish: 31-03-2012

Prediction of phase equilibria involving phase transfer catalyst

Phase transfer catalysis (PTC) has the potential to stand out as an attractive alternative to conventional processes for the synthesize of special organic chemicals, from two immiscible reactants, that normally will not contact each other: in PTC systems a phase transfer catalyst acts as a shuttle between a polar phase that contains the salt reactants and a non-polar phase that contains the organic reactants. Many factors affect PTC process yields and kinetics: choice of the organic phase, choice of the catalyst, presence of extra ionic species, temperature, stirring rate. The aim of this project is to enable semi-quantitative and quantitative estimations of phase equilibria involving PTC and, ultimately, to develop a systematic methodology to select the best system features and operating conditions for a given synthesis. This screening strategy should take into account the knowledge gained from data and model-based analysis of solubility and phase equilibria of the reacting systems.

Keywords: *Phase transition catalysis; solubility modelling; phase equilibria modelling; solvents*

Ravendra Singh (RS)

Supervisors: RaG, KVG, JW
Started: 01-09-2009
Finish: 28-02-2011

Systematic framework for design and adaption of "Flexible, Fast, and Future - F^3" production processes

The objective of this project is to develop a systematic framework and a generic "Substrates Adoption" methodology through which a fast and flexible continuous modular plant (F^3 plant) can be designed and adapted for a series of similar substrates or changes in the F^3 plant. The changes can be related to process operational conditions as well as in the physical arrangement of the process equipments. The supporting tools for the substrates adoption are: (1) a knowledge base consisting of the properties of substances (reactants, products, reagents, solvents, and catalysts), reaction characteristics and characteristics of unit operations; and (2) a model library consisting of the thermodynamic models and process operational models. The systematic framework, the methodology and the supporting tools have been developed and their scope and significance have been demonstrated through a conceptual example.

Keywords: *F^3 factory; substrate adaption methodology; modelling; knowledge-base; pharmaceutical industry*

Publications: PEC09-05; PEC09-71; PEC09-73

Ricardo Morales-Rodriguez (RMR)

Supervisors: GSI, AM, KVG
Started: 01-06-2009
Finish: 31-05-2010

Integrated modelling for simulation and design of novel enzymatic processes

The project aims at understanding the dynamic interactions among different unit operations involved in bioethanol production for purposes of better design and control. An integrated dynamic modelling framework (IDMF) for 2nd generation bioethanol production has been developed, and consists of: collection, analysis and identification of dynamic mathematical models to represent the diverse unit operations involved in the process. Different process configurations are studied in through one modelling and simulation platform (MatLab/ Simulink). The IDMF is used to investigate the interactions among the different units having different operating strategies; the implementation of appropriate controllers suitable for their guaranteed optimal operation; to identify new avenues for improved biofuels processing strategies using lignocellulosic feedstock; and for providing operator training in the plant.

Keywords: Integrated dynamic modelling framework; bioethanol production; lignocellulosic feedstock

Publications: PEC09-38; PEC10-22

4. CAPEC Software

Development of CAPEC software is closely related to the CAPEC research projects. Since a majority of CAPEC research projects deal with the use of computers to solve process/product engineering problems, the theories and algorithms developed in the research projects are validated through these computer programs. Among these, the computer programs that have a general appeal with respect to their application and do not have any restrictions imposed by a consortium member company, are collected and distributed as part of the CAPEC software. CAPEC software is not a commercial software and are distributed exclusively only to the CAPEC industrial consortium member companies. A special version is distributed at a nominal price for educational purposes.

The objective of the CAPEC software is to promote the use of computer aided methods and tools developed by CAPEC in the solution of current and future process/product engineering problems. The CAPEC software consists of the following:

- Integrated Computer Aided System – ICAS
- EXCEL based macros (ProPred, CAPECDB Manager)
- Continuous Time Stochastic Modeling – CTSM
- UNIFAC-Utility (group definitions, VLE database, etc.)
- Grid of Linear Models – GoLM
- Special Software (ICAS-PAT, SustainPro, *v*PPD-*Lab*)
- PC-SAFT software package (beta-version)
- SMSWIN – A tool for properties and phase equilibrium calculations, especially suitable for solid-liquid systems (compliments with the features in ICAS)

4.1 Integrated Computer Aided System – ICAS 13.0

ICAS combines computer-aided tools for modelling, simulation (including property prediction), synthesis/design, control and analysis into a single integrated system. These tools are present in ICAS as toolboxes. During the solution of a problem, the user may move from one toolbox to another to solve problems requiring more than one tool. For example, in process synthesis, one option is to define the feed stream, then analyse the mixture (analysis and utility toolbox), then generate a flowsheet (synthesis toolbox), then optimise the flowsheet (design toolbox), and finally verify the design (analysis toolbox). From any toolbox it is possible to invoke the simulation engine to perform steady state and/or dynamic simulation for batch and/or continuous process operations. From the synthesis toolbox, it is possible to invoke the solvent design tool (in design toolbox) if a solvent is needed for a specific separation task. There is also a utility toolbox, which determines properties, phase diagrams, etc., which can be used by the other toolboxes or by the user to analyze the behaviour of the specified system. “ICAS documentations” provides information on installation of ICAS, tutorials at basic and advanced levels and other useful information such as a list of dll-files copied during installation and new features of the latest version of ICAS. Figure 4.1 highlights the idea of integration and the advantages that can be obtained through this integration.

In ICAS 13.0, new features have been added to the following tools: ProPred (pure component property prediction), MoT (modelling toolbox), ProCamd (computer aided molecular design), and the CAPEC-database. The EXCEL based macros (ProPred and

CAPECDB manager) have been updated with new features and corresponding manuals. The CAPECDB manager also includes an azeotropic data collection and analysis feature. In addition, three special software (EXCEL based): Sustain-Pro, ICAS-PAT and the Virtual PPD-lab (*v*PPDL) have been revised and improved. Each of these software, use a number of ICAS tools and models generated through MoT. For a list of ICAS tools, see ICAS Documentation or the ICAS poster. A number of new properties for organic chemicals as well as polymer repeat units have been added to ProPred. In ProCAMD, it is now possible to design the polymer repeat units as well as check for target properties of generated structures through ProPred.

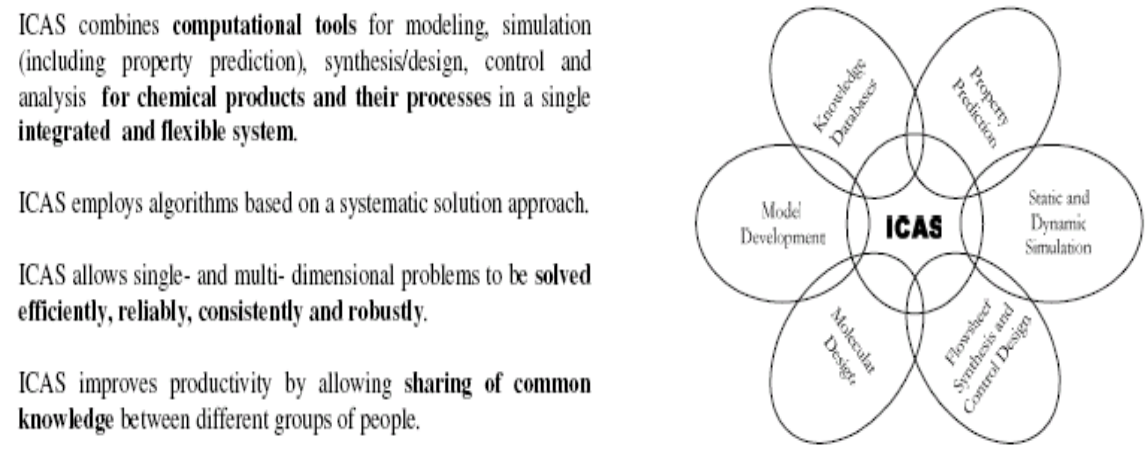


Figure 4.1: The idea of integration within ICAS

In general, ICAS 13.0 has become a much more robust and reliable version of ICAS with a wider application range. Finally, new additions to ICAS documents related to ProCAFD and Batch-Dis can be found after installation of ICAS under the examples-directory. New versions of manuals for the following tools in ICAS are also available - ProPred, MoT, SoluCalc and ProCamd. After installation of ICAS, users will find a number of worked out examples given in the “examples” and “tutorials” directories. Figure 4.2 highlights the new features in ICAS 13.0 while Fig. 4.3 highlights the work-flow in the implementation of a model (starting from transferring the published model equations to MoT and ending with a COM-object that can be executed from different external software).

In ICAS 13.0, MoT has new features (see the MoT new features document); ProCamd and ProPred have had bug-fixes; and the CAPECDB (EXCEL version) has a new solvents database added to it. Also, SustainPro and the virtual product-process design lab are new versions.

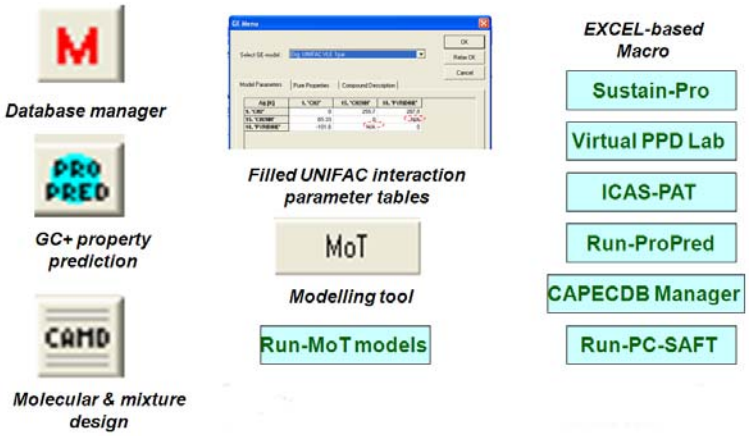


Figure 4.2: Highlight of new features in ICAS 13.0

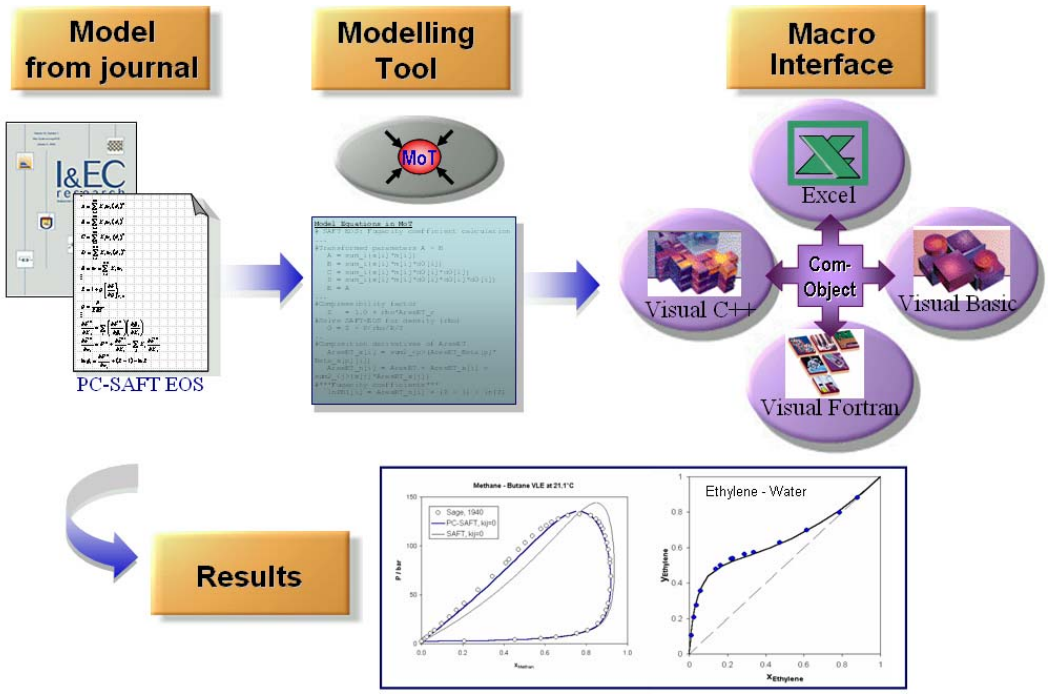


Figure 4.3: COM-object generation through MoT and use in external software

4.2 EXCEL based macros (ProPred, CAPECDB Manager)

Two EXCEL based software has been developed to further facilitate the use of ICAS-ProPred and the CAPEC-database. EXCEL-ProPred, the user opens the EXCEL macro and then performs different property calculations through ProPred. Here, the EXCEL spreadsheets become the working area and ProPred is the property calculator.

In the CAPECDB Manager, the EXCEL macro helps the user in the search for data available in the CAPEC database. A new feature to this database is the availability of azeotropic data. A solvents database consisting of information on approximately 1400 solvents has been added.

4.3 Continuous Time Stochastic Modeling - CTSM

Continuous Time Stochastic Modelling means semi-physical modelling of dynamic systems based on stochastic differential equations. Stochastic differential equations contain a diffusion term to account for random effects, but are otherwise structurally similar to ordinary differential equations. This means that conventional modelling based on the principles of physics can be applied to set up the model structure.

With the model structure given, CTSM provides methods for estimating any unknown parameters of the model from time series data, including the parameters of the diffusion term. These methods are able to handle both linear and nonlinear models, and the program also provides great flexibility with respect to the data that can be used, *e.g.* by allowing varying sample times, missing observations and occasional outliers.

The methods implemented in CTSM are a *maximum likelihood* (ML) method and a *maximum a posteriori* (MAP) method. With both methods the program provides the ability to use several independent data files, just as it is possible to estimate initial conditions, if these are unknown. The ML and MAP methods are both sound statistically based estimation methods, which means that once the parameters have been estimated, statistical tests can easily be performed to test the validity of the corresponding model. Some such test features are included in CTSM and others will be included at a later stage. The new version of CTSM is 2.2, which has a graphical user interface for setting up models, estimating parameters and generating validation data. This new version has an improved solution of the stochastic differential equations by using a stiff numerical integration routine. Furthermore the flexibility in applying the uncovering of too simply modelled functionalities has been increased, among others by enabling much simpler modification of the models. These modifications are needed for revealing unknown functionalities from experimental data.

4.4 UNIFAC-Utility

KT-UNIFAC-utility is a program that helps the user to check the consistency of UNIFAC groups, their parameter values and the representation of the molecules with the UNIFAC groups. For a specified mixture, the program determines the UNIFAC group information and passes the relevant data to ICAS for use in TML and other tools.

4.5 Special ICAS-based software (ICAS-PAT, SustainPro, vPPD-lab)

4.5.1 ICAS-PAT

ICAS-PAT is an EXCEL based software that designs and/or analyzes a process monitoring system, given the process information. It has a built-in knowledge base of information about process operations, the variables that need to be measured, the variables that need to be monitored and the equipments that could be used. It also has a library of models that may be needed to supplement the data available for the process under investigation. The library models are run through ICAS-MoT. The EXCEL macro guides the user through an established work-flow based on the systematic methodology developed by Singh et al. (see PEC08-05). A manual and several solved case studies are available. Figure 4.4a highlights the main features of ICAS-PAT.

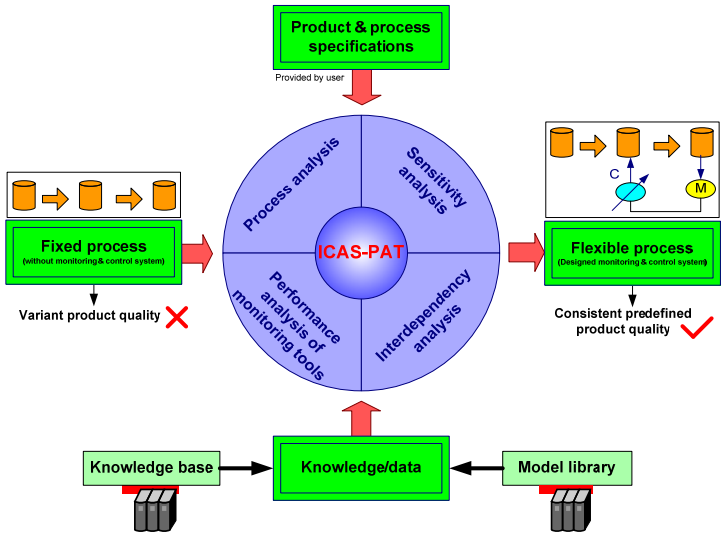


Figure 4.4a: Overview of the main features of ICAS-PAT.

4.5.2 SustainPro

SustainPro is an EXCEL based software, which provides options for retrofit analysis and performance analysis of a given process. As highlighted in Fig 4.4b, the inputs to *SustainPro* are the mass and the energy balance data that can be collected either from the plant or from process simulations. To perform the retrofit analysis, *SustainPro* also requires as input, several cost related data (the prices for utilities, the prices for chemicals, etc.). *SustainPro* is able to read the mass and the energy balance from an EXCEL file generated by a commercial simulator. The EXCEL interface guides the user through the steps of the work-flow (solution steps). After applying all the steps *SustainPro* gives as output for the retrofit analysis, a new design alternative suggestion for improving the process being investigated. When the software is used for performance analysis, the output provides the calculated values of the sustainability metrics and the safety indices. As it can be seen from Fig 4.4b, the two options can be combined, which means that they complement each other. After applying the retrofit analysis, the performance analysis is performed and compared with the base case design.

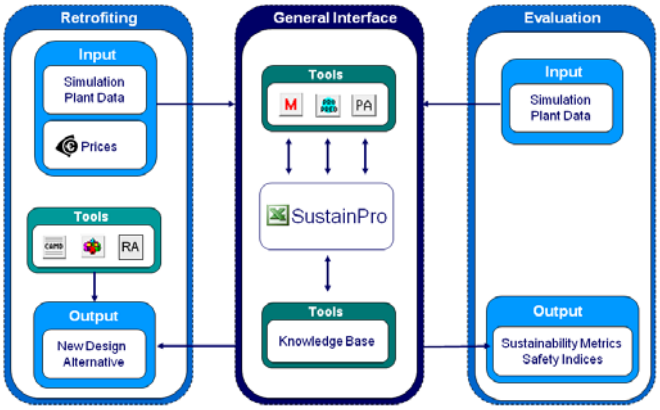


Figure 4.4b: Overview of the main features of SustainPro

4.5.3 Virtual Product-Process Design Lab

The idea behind the virtual product-process design lab is the following: instead of doing the experiments needed to search for a product and its process to manufacture it, the engineer/scientist performs *virtual* experiments, through the *v*PPD-lab software. The software therefore contains a large knowledge base of data (of chemicals, of solvents, of plants, of microcapsule devices, etc.); a large collection of models (models for property prediction, models for controlled release, models for mixing, etc.); of design algorithms (methods for formulation design, methods for molecule design, methods for polymer design, methods for process flowsheet synthesis, etc); other tools (property prediction software; model generation software; equipment design software; design of experiments software, etc.). All of the above are organized through a framework for efficient management of the complexity. Figure 4.4c gives an overview of the main features of the *v*PPD-lab software, which has been used in the design and evaluation of the controlled release of a drug active ingredient (codeine) through a polymeric microcapsule. In the first step the problem is defined (identity of the active ingredient; the desired controlled release parameters, etc., are given in the "documentation" box of *v*PPD-lab). In the second step the selection of the application source (codeine released into the body), the primary properties of solvent and the polymer (needed by the controlled release model) is made (if the user is unable to provide this information, methods for solvent design and polymer design are used to generate a list of candidates to select from). In the next step the selection and calculation of the functional properties needed to evaluate the controlled release design is made (if models are not available, the modelling software helps to generate new models). In the next steps, the product performance model is used to predict the product behaviour. If the desired (target) performance is matched, then the last step of verifying the product performance through experiments is performed. If the target is not matched, it is possible to repeat from any of the earlier steps with a new design alternative. An option for formulation design together with the associated databases has been added.

Important issues to note from this example are that multi-scale models have been used, data and knowledge from different disciplines have been used and, design/evaluation problem has been effectively used by solving a collection of sub-problems according to a pre-determined sequence. The final step (not shown) would be to select a few of the alternatives and perform the necessary experiments to validate the selection. Therefore, the experiments are done not to design the product but to verify the product. This approach has the potential to save time and money in bringing a chemical based product to the market. Obviously, the accuracy and range of application of the *v*PPD-lab software depends on the available data and models in the software.

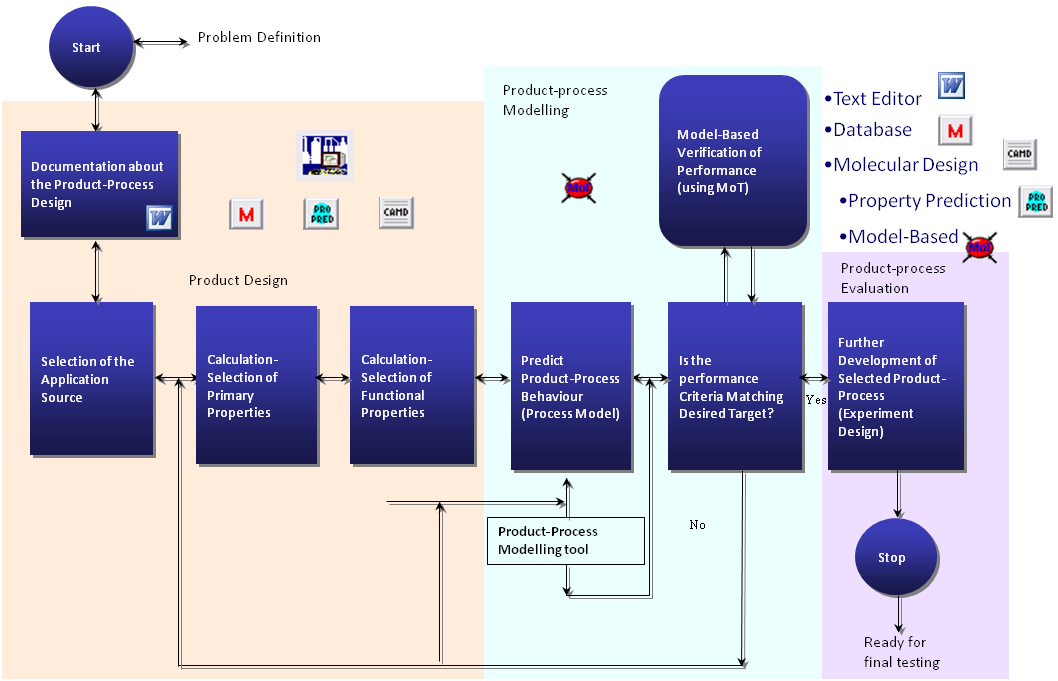


Figure 4.4c: The virtual product-process design lab

4.6 PC-SAFT Software Package (beta-version)

This software performs multicomponent phase equilibrium calculations at given temperature with the PC-SAFT equation of state.

- The user firstly provides some information about the molecules involved in the mixture and gives the molar fraction of each of them. The temperature of the mixture is also required. Molecules may be chosen from an extended databank of nearly 1000 compounds (including some polymers) or may be created from GC^+ methods.
- Once the mixture completely described, the user chooses between two kinds of calculations:

[1] *bubble point calculation:* The mixture is assumed to be a saturated liquid. The software calculates the bubble pressure and the composition of the vapour phase in equilibrium (a single bubble in this case).

[2] *dew point calculation:* The mixture is assumed to be a saturated vapour. The software calculates the dew pressure and the composition of the liquid phase in equilibrium (a single droplet in this case).

4.7 SMSWIN

SMSWIN is a software package that Syngenta has given to CAPEC for maintenance, further development and integration with ICAS. SMSWIN has a database of compounds and their properties, a collection of property models for phase equilibrium calculations, which are especially suitable for solution properties involving solids. Currently, ProPred and the KT-UNIFAC model have been integrated with SMSWIN.

5. Research highlights (2009-2010)

The research highlights are discussed below in terms of new developments as well as publications record.

5.1 Summary of completed PhD research projects

5.1.1 Computer aided design and analysis of reaction-separation and separation-separation systems - Kavitha C Sataynarayana (PEC09-35)

This thesis describes the development of a systematic multiscale framework for the design of polymers. This involves the initial design of the polymer repeat unit structures using computer aided molecular design (CAMD) techniques based on a reverse problem formulation. Two important efforts go behind building the methodology for the design of polymer repeat unit structures using CAMD – (a) property model development and (b) modification of an existing multi-step and multilevel CAMD algorithm. The properties of the polymer repeat unit structures are predicted using the group contribution method proposed by Marrero and Gani method. In case of any missing group or missing group contribution, which are the main limitations of any group contribution method, the missing group parameters are estimated using an atom-connectivity index method developed in this project. Thus, the group contribution plus (GC+) property models, being the first of its kind to integrate the group contribution approach (Marrero and Gani; Van Krevelen) and the atom-connectivity index approach (Bicerano) to polymers have been developed in this work with a reasonable statistical accuracy. Decreasing the time spent on computational aspects of the model development is explored by using OfficeGRID, a grid technology based application. The multi-step and multi-level CAMD algorithm (proposed by Harper), which can handle the combinatorial explosion problem while generating polymer structures, is modified in this work to generate polymer repeat units; predict the properties of the generated structures using the GC+ property models and screen the polymer repeat unit structures for the specified set of structural and property constraints. The result is a modified multi-step and multi-level algorithm (using GC+ methods), capable of handling a large number of polymer repeat unit structures even if some group parameters are not be available.

The developed property models and the modified CAMD algorithm are automated by incorporating them in ProPred, a in-house property prediction software as well as in ProCAMD, an in-house CAMD based software. The developed methodology for the design of polymer repeat unit structures based on the specified structural and property constraints have been tested in a series of case studies. Traditional CAMD can only design the polymer repeat unit structures. It cannot consider the optimal arrangement of repeat units or chain length effects. In this context, the methodology for the polymer repeat unit design is extended to the design of the polymer chains using the atomistic or molecular modelling approach. This extended methodology is also tested on a case study in this thesis. Thus, the use of the reverse problem formulation - combined with grid technology - for polymer design has been combined with molecular simulations. While this application of the reverse problem formulation incorporates elements of multi-scale product design, the full integration of the reverse problem formulation into the complete multi-scale framework has yet to be achieved.

5.1.2 Model-based retrofit design and analysis of petrochemical processes - Jamal El Bashir Ali Rashed (PEC09-36)

Technological, economical and new environmental regulation changes have an important impact on the petrochemical processing industry. As a result, many of the existing production processes require constant improvements through retrofitting that are available by generation of new alternatives to the process that exhibit improvements on design parameters such as operability, cost, waste reduction and environmental impact.

This project presents the development of a systematic methodology plus its associated algorithms for generation and screening of feasible retrofit process alternatives, to produce the same products from the same raw materials and from them, to identify the more sustainable ones. The methodology is organized in three stages: 1. Targeted process analysis; 2. Reverse process synthesis and design; and 3. Final selection and verification. In the first stage, the process flowsheet is analyzed in order to identify the design/operational weak points, indicating potential for improvement and thereby to set design targets that may improve the process. In the next stage, the identification of feasible process options is made, based on thermodynamic insights. The process options are generated through an analysis of the physico-chemical properties of the particular mixture present in the system and based on the relationships between properties and separation techniques, a list of feasible alternatives for the particular separation task is generated. A reverse approach is used to identify and match the final design details for process options. According to the reverse approach, the design variables that match the specified process targets for each unit operation in the process are determined by solving a new class of unit operation models based on the driving force that "drives" the operation. First, the driving force needed to convert a given feed stream to the desired product streams, is calculated. Next, the variables (design) through which the calculated driving-force can be matched, are determined. Driving force based models are developed for application in different separation and reaction processes in model based retrofit methods for design and analysis of petrochemical processes. In the third stage (final verification stage), performance of the identified feasible process alternatives are compared, for final selection, in terms of sustainability metrics.

Application of the developed methodology has been illustrated through three case studies from the petrochemical industry. The first case study deals with the tert- amyl-methyl ether (TAME) production process. The second case study concerns the styrene production process and the third case study deals with the separation of isobutyl alcohol and isobutyl acetate.

5.1.3 Model-based computer aided framework for design of process monitoring and analysis systems – Ravendra Singh (PEC09-47)

In chemicals based product manufacturing, as in pharmaceutical, food and agrochemical industries, a well-designed process monitoring and analysis system (PAT system) plays a very important role. These PAT systems ensure that the chemicals based product is manufactured with the specified end-product qualities. Systematic computer-aided methods and tools provide the means to design the necessary process monitoring and analysis system and/or to validate any existing process monitoring and analysis system.

In this PhD-project a generic model and data (knowledge) based computer-aided framework for including the methods and tools through which a process monitoring and

analysis system for product quality control can be designed, analyzed and/or validated, has been developed. Corresponding software has been developed as well.

Two important supporting tools developed as part of the framework are a knowledge base and a model library. The knowledge base provides the necessary information/data during the design of the process monitoring and analysis system while the model library generates additional or missing data needed for design and analysis. The developed design methodology consists of nine hierarchical steps for design of a process monitoring and analysis system. These steps cover problem definition, analysis (process, sensitivity, interdependency), design and verification of the PAT system. The developed framework and methodology has been implemented into a software (ICAS-PAT) that has made the use of the PAT design procedure easy, consistent and fast. Some additional features have also been added to the ICAS-PAT software that has made it more useful and user friendly. For example, the options to open and analyze stored solved examples, to find the different applications of any monitoring tools, to search the knowledge/data stored in the knowledge base, to draw the open and closed-loop process flow diagrams and to build reports in MS word for documenting the design of a process monitoring and analysis system. To demonstrate the wide applicability of the developed framework, methodology and corresponding software (ICAS-PAT) in pharmaceutical, biochemical and food production processes three case studies involving a tablet manufacturing process, a fermentation process and a cheese manufacturing process have been developed.

5.1.4: Design of sustainable chemical processes: Systematic retrofit analysis, generation and evaluation of alternatives – Ana Carvalho (PEC09-62)

This thesis presents a new generic and systematic methodology to design new sustainable alternatives for any chemical process. The methodology uses a set of indicators to identify the critical points in the process. The indicators with the highest potential for improvements are identified and then selected to generate the new design alternatives. The new design alternatives are evaluated through the use of performance criteria parameters (sustainability metrics and safety indices). A software, called *SustainPro,* has been developed and performs the whole methodology.

Nowadays the concerns about the future of humanity are growing due to an increase of environmental problems, the depleting of natural resources as well as the social effects generated because of industrial activity. Consequently, one issue that has gained importance is Sustainability. It is possible to define sustainability as a development strategy that meets the needs of the present without compromising the ability of future generations to meet their own needs. One way to apply this strategy to industry is to retrofit the processes by generating new process/ operation alternatives. These alternatives will integrate the economic, the environmental and the social aspects into industry production. All the previous factors have motivated the development of this methodology and the respective software. With this work, it is now possible to analyse and consequently generate new sustainable alternatives in any chemical process operating in batch and continuous mode that improve the aforementioned concerns.

The software allowed a more precise and faster analysis that can be reproduced by any person at any time. The methodology and the software were highlighted through the use of case studies using processes operating in continuous and batch mode. Some of those the data was collected from real plant.

5.1.5: Development of group contribution^{plus} models for prediction of properties of organic chemical systems – Merlin Alvarado-Morales (PEC10-13)

This PhD-project was concerned with the development and application of a framework for synthesis, design and analysis of chemical and biochemical processes. The developed framework addressed the formulation, solution, and analysis of the synthesis/design problem through a systems approach where emphasis was given on the use of the process-group contribution based methodology. This methodology helps to generate and test process flowsheet alternatives in a truly predictive manner, in the same way, molecules are designed through group contribution based computer aided molecular design.

The three fundamental objects of the PGC-methodology are the process-groups (building blocks) representing process unit operations; connectivity rules to join the process-groups, and the flowsheet property models to evaluate the performance of the generated flowsheet structures. In order to extend the application range of the PGC methodology, a set of new process-groups together with their specifications have been developed. The synthesis of the chemical and biochemical process flowsheets has been performed through the reverse property approach, where the process-groups are combined to form feasible flowsheet structures having desired (target) properties. The design of the most promising process flowsheet candidates is performed through the reverse simulation approach, where the design parameters of the unit operations in the process flowsheet are determined from the specifications of their inlet and outlet streams inherited from the corresponding process-groups. The reverse simulation methods supporting the framework are based on the attainable region (AR) and the driving force (DF) concepts, which guarantees a near optimal performance design with respect to selectivity for reactor units and with respect to energy consumption for separation schemes.

The framework for synthesis and design of chemical and biochemical processes together with the models, methods and tools is generic and can be applied to a large range of problems, either to improve an existing process flowsheet or to design a new process flowsheet. The developed framework and associated computer aided methods and tools have been tested using a series of case studies, for example, the production of ethanol, succinic acid and diethyl succinate from renewable resources.

5.2 Publications record

The last 12-months have seen a big increase for CAPEC in the number of peer-reviewed journal publications. 37 published paper from 2009 to present (plus 24 “in press” or “submitted”) have been published in major chemical engineering journals (see Appendix 7.3). There have been 10 plenary or keynote lectures international conferences and 104 presentations have been made in important international conferences. This has given CAPEC greater visibility and attracted more attention to the research results published by CAPEC coworkers. CAPEC continues to have an open policy with respect to the publication of model parameters (especially, the CAPEC developed property models). The new version of ICAS 13.0 has all the latest property models and updated property model parameters.

6. Future Developments & Opportunities

Process systems engineering promotes the solution of a problem in a systematic manner. In this way, although it has traditionally been applied by the chemical engineering community to solve problems for the oil and petrochemical industries, its potential application range is much wider. This is because the word "process" also implies, among others, the process of solving a problem; design of a biochemical / biological process for conversion of biomaterial to specific chemicals; and, the process of finding/designing chemicals with desired properties.

Most of the earlier developments can be linked to chemical processes involved with the manufacture of high volume bulk chemicals and the related industries (such as the oil and gas, petrochemical and chemical industries). To a lesser extent, these methods and tools have also been applied to the manufacture of low volume specialty chemicals. Since its formation, CAPEC has contributed by providing systematic, reliable and efficient models, methods and tools that have now become standard for the chemical process industries as well as in chemical engineering education. CAPEC software, employing CAPEC models and methods, such as ProPred (property prediction software), ProCAMD (molecular design-solvent selection software), SustainPro (sustainable process design software), ProCAFD (process flowsheet design/synthesis), ICAS (Integrated Computer Aided System), are routinely used by the CAPEC consortium members and more than 50 universities outside of Denmark.

The question therefore arises, what next? Where are the new challenges for CAPEC and what could be the new directions for research and education? Through collaboration with the CAPEC industrial member companies and academic partners, CAPEC conducted a "gap-analysis" with respect to identifying the current trends and the future needs with respect to chemical products, the processes that manufacture them and the models, methods and tools needed to design, analyze and operate them. The conclusions are briefly summarized below.

"*To satisfy the needs of the modern society, it is necessary to continuously develop better and significantly improved chemicals based products. The bulk chemicals as well as the specialty chemicals have important roles. For example, the bulk chemicals act as raw materials, solvents, process fluids, etc., are needed in the manufacture of specialty chemicals that may become an active ingredient for a pharmaceutical and/or drug product. Therefore improved designs of continuous processes (needed for the manufacture of bulk chemicals) are as important as designs of batch operations (needed for the manufacture of specialty chemicals). Also, alternative production routes from renewable feed materials and retrofit of processes for changes in feed materials while focusing on energy, water and environmental issues will need special attention.*"

Based on the above, CAPEC's future research will address the following questions:

- How does one identify the chemicals and their synthesis routes that will help to meet these demands, taking into account, also the questions of sustainability and protection of the environment (*eg.*, energy conservation and water resources)?
- How does one find their replacements and the processes to manufacture them? The sources for many of the raw materials used, especially those derived from oil, gas, and

some plants/animals continue to be depleted and may soon be economically infeasible to use (*eg*., bio-refinery and green chemistry).
- How to develop and provide the necessary models, methods and tools through which the future problems can be addressed (*eg.*, multiscale modelling & integration/intensification)?

Based on the above and new developments at the department of chemical and biochemical engineering at DTU, has resulted in establishing a stronger collaboration between the centers CAPEC and PROCESS. The two centers have several joint post-doc, PhD and MSc-level projects. Also, it has been decided that the results from these joint projects will also be available to the industrial consortium members. Thus, CAPEC and PROCESS plans to invest heavily in the following areas:
- Development of a generic computer aided modelling framework through which models of different forms and scale can be generated/created with significantly less time and resources than current practice.
- Use of a multidisciplinary approach because the process-product knowledge (including data) will come from different sources and the performance criteria, factors, etc., will involve other research groups (expertise). The opportunity for CAPEC and PROCESS is that it can play the role of the "integrator" or "glue".
- Develop systematic solution approaches that combine methods and tools from different sources into problem specific flexible, reliable and efficient systems.

More specifically, for CAPEC and PROCESS to meet the challenges for the future, the following topics will have higher priority:
- computer aided frameworks for generation and use of multi-scale models (further extension of the predictive-generic property-product–process models)
- methods for design of experiments to collect and analyze data (efficient use of resources in data collection) and, verification by experiments (through collaboration with PROCESS)
- methods & tools for process-product monitoring/control systems (and their design)
- sustainable process-product development (such as, hybrid processes, green chemistry, process intensification)
- systematic methods for product discovery (further extension of computer aided molecular and mixture design)
- Evaluation of alternative processes for sustainability, retrofit and process modification
- Evaluation tools to identify (bio-) catalyst bottle-neck and strategies to improve the (bio-) catalyst.

6.1 Managing the complexity through a systems approach

Product-process design and development in the life sciences, pharmaceutical, food and related industries, as opposed to the oil and petrochemical industries, is principally dependent on experiment-based trial and error approaches. Furthermore, unlike the oil and petrochemical industries in the life sciences, pharmaceutical, food and related industries, problems associated with product-process design and development involve, among others, the following distinct features:

- Multi-scale: important data related to the chemicals come from different sources, at different scales of time and size; for example, the properties that define the product characteristics are based on the microstructure of the molecule or material, while the process behaviour that needs to be monitored and controlled during operation is defined by the macroscopic (end-use) properties of the chemical system.
- Multidiscipline: the conversion of the biomaterial through biocatalysis requires knowledge of organic synthesis, enzymes, reaction catalysis, bioreactor design and operation – information about these topics come from different disciplines.
- Computer-aided techniques: lack of models to predict the behaviour of the chemicals at different scales, of enzymes during organic synthesis, of reaction kinetics, etc., means that appropriate model-based computer aided techniques have not been developed and use of experiment-based techniques is the only option.

Advances have been made on each of the above issues on specific areas of chemical and biochemical engineering. For example, multiscale polymerization reactors have been developed to investigate the operation of reactors; techno-economic assessment related to sustainability biofuels have been made using data from engineers, economists and scientists; computer-aided systems have been developed to perform routine mass and energy balances of chemical and biochemical processes. The demand for improved chemical-based products, made from more sustainable raw material resources and employing more efficient processes to make them, however, requires the above issues and others to be tackled in an integrated manner. This means that methods and tools suitable for current and future product-process development need to manage complex situations that require handling of data and knowledge from different sources and at different time and size scales. That is, the dimensions of the problems we need to solve have become larger. Therefore, a systems approach that can efficiently “manage the complexity” becomes very desirable.

The multi-dimensional and multi-scalar nature of problems is highlighted through Fig. 5.1, where, it can be noted that at the micro- and meso- scales, the related problems are dealing with the microstructure of the molecules or materials and their properties; at the macro-scale (traditional area of application of chemical engineering), the related problems are mainly dealing with the process and its operation to produce a desired chemical; at the mega-scale, the related problems are, among others, dealing with enterprise wide optimization and supply chain issues. Many of the problems of current interest, such as, finding the optimal biorefinery, sustainable chemical process-product design, use of green solvents, process (energy and water) integration, etc., involve the macro- and mega-scales.

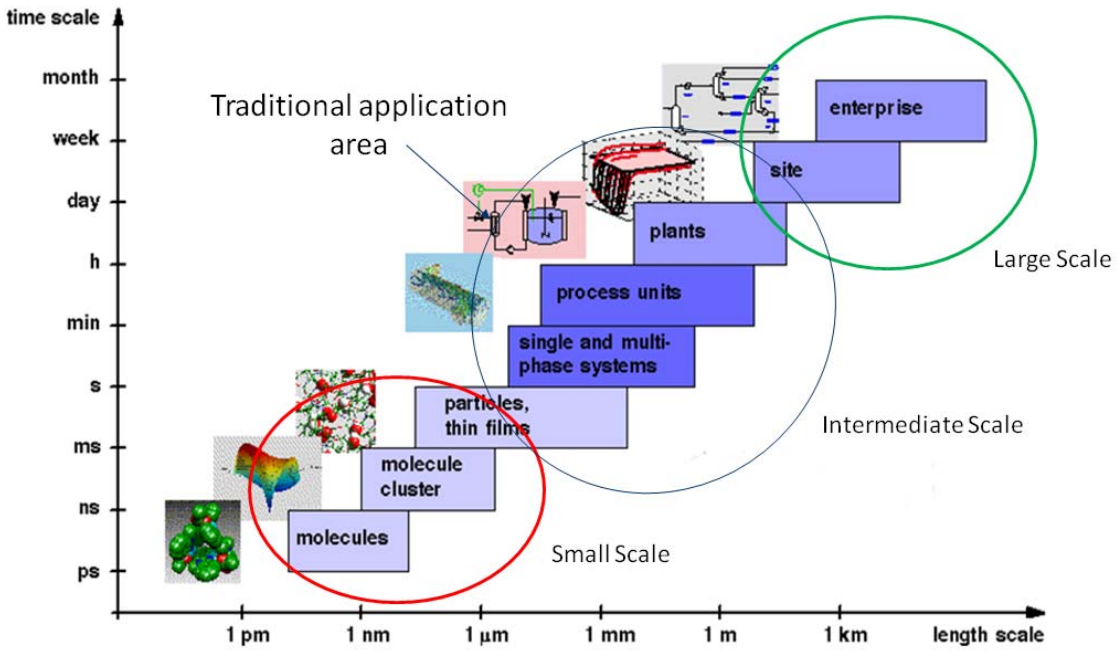


Figure 5.1: Multiscale nature of product-process design problems

To manage the complexity, a systems approach would develop a framework (the architecture of the software) for handling the diverse set of methods and tools needed to solve a wide range of problems, for a potential computer-aided system. Such systems need to have a knowledge base of data (for example, of the active ingredients, solvents, polymers, etc.); a library of models (for example, models to predict properties – in case data is not available - of active ingredients, solvents, polymers, etc.; models to predict the controlled release from the microcapsule; models to predict the behaviour of the mixing process); a design method (for example, guiding the engineer/scientist through the sequence of steps needed to identify the best solution); and, other associated methods-tools (such as a tool to analyze data; a tool to create the missing model; a tool to screen feasible alternatives). The principal idea here is to decompose a complex problem into a set of sub-problems that are easier to solve and identify those that can be solved through model-based solution approaches. Solving these sub-problems according to a pre-determined sequence helps to reduce the search space through each subsequent sub-problem solution, until a sub-problem cannot be solved with models anymore. At this point, the experiment-based trial and error approach takes over to determine the final solution. The advantage of this combined hybrid (systems approach) is that during the early stages, where enough data and models are available (or could be easily generated), the search space is rapidly reduced. In the later stages, where quantitative values become important and data/models become more unreliable, the experimental resources are employed, sometimes only to evaluate a few feasible alternatives to identify the truly innovative and best solution. Several examples of such computer aided systems can be found at CAPEC and current research is expanding on this approach through the development of a collection of methods and tools.

6.2 Some specific plans (CAPEC coworkers) for the future

Within the next 6-months, CAPEC and PROCESS plan to jointly start 3-4 PhD projects in the areas of energy and environment; product-process design; multiscale modelling

(crystallization); (bio-) process modelling, design, control under uncertainty; solvent based organic synthesis; and environmental issues (autotrophic nitrogen removal – 2 PhD projects; one to start from September 2010). Also, 2 post-doctoral projects will be started in the area of property modelling (Elisa Conte) and, process-product synthesis (NN). Also, several new MSc-level projects on computer-aided product design (crystallization); solvent-based product design; energy and environment; design under uncertainty; sustainable process design; micro-reactor fermentation; cellulose hydrolysis kinetics; and uncertainty quantification in property prediction will be started within the next 6-months.

7. Appendix

7.1 Membrane lab

List of experiments:

Experiment Type	Experiment objective (measure)
Pressure driven	Water permeability
	Solute permeability
	Membrane selectivity/retention
	Gas permeability
Concentration driven	Osmotic water permeability
	Solute permeability
	Time-lag measurements and/or sorption-desorption measurements (diffusion coefficients, distribution coefficients)
Partial pressure driven	Water (vapor) permeability
	Solute (vapor) permeability
	Concentration factor/separation factor
Electrical potential driven	Electrical permeability/resistence
	Solute permeability
	Electro-osmotic water permeability

List of equipments:

Type of equipment	Remarks
Various flat sheet flow cell plants	Pressurized cells for nano-filtration (NF), ultra-filtration (UF), micro-filtration (MF), reverse-osmosis (RO)
	Diffusion and reverse osmosis cells
Ultra-filtration/micro-filtration hollow fiber module plants	High frequency back-pulsing operation
	High frequency vibration operation
Electro-ultrfiltration test plant	
Lab-20 pilot module	For RO, NF, UF, MF
M38/M39/4” – spiral wound module	DSS
Membrane distillation test plants	Pervaporation, vacuum membrane distillation
	Direct contact membrane distillation, sweeping gas membrane distillation, osmotic membrane distillation
Test cells	Electrodialysis
Pilot plant	Electrodialysis
Casting equipment	Membranes
Modification equipment/machine	UV
Analytical instruments	*HPLC/SEC with RI and UV detectors*
	Conductivity meters
	Polarimeter
	UV instrument

7.2 CAPEC Control Lab

The main purpose of the CAPEC Control Lab is to give our students hands-on experience with process control problems. The laboratory is presently undergoing a complete renovation.

Two facilities are in use:

- a 4-tank exercise, and
- a distillation column

With the 4-tank exercise (used as a 2-tank system), students make two experiments. The first day they determine the dynamics of the system. Then they go to the computer lab to configure a PI-controller by simulation. On the second day they try out their controller settings on the real system. This setup is used in all our introductory teaching; about 75 students each year.

A HTST pasteurizer has also been established

The distillation column is used in an intensive 3-weeks course. This course teaches the participants to:

- Plan and execute start-up of the chemical plant.
- Apply a Distributed Control System for chemical plant operation.
- Simulate and document the operation of a chemical plant.
- Reason on process behaviour during start-up and operation.

4 tank exercise

HTST pasteurizer

Indirect Vapour Recompression Distillation Pilot Plant

7.3 Publication list (2009-2010)

Publications listed under PECxx-yy indicate CAPEC publications where one or more authors are CAPEC members, whether or not PROCESS is involved. Publications listed under PROCESS indicate PROCESS publications where there is no joint activity with CAPEC.

	A - Ph.D. Theses and Monographs
PEC09-01	Maria Antonieta Alvarez Villanueva, Stuart M. Stocks and Sten Bay Jørgensen, 2009, "Bioprocess Modelling for Learning Model Predictive Control (L-MPC)", in: "Computational Intelligence Techniques for Bioprocess Modelling, Supervision and Control", M.C.Nicoletti and L.C. Jain (Eds.), Studies in Computational Intelligence, Springer-Verlag, Germany, Chapter 9, pp. 237-280
PEC09-16	Ricardo Morales Rodriquez, 2009, "Computer-Aided Multiscale Modelling for Chemical Product-Process Design", Ph.D. thesis
PEC09-17	Hugo Edson Gonzalez Villalba, 2009, "Development of Group Contribution^{plus} Models for Properties of Organic Chemical Systems", Ph.D. thesis
PEC09-35	Kavitha Chelakara Satyanarayana, 2009, "Computer-aided polymer design using Multiscale modeling", Ph.D. thesis
PEC09-36	Jamal El Bashir Ali Rashed, 2009, "Model-based retrofit design and analysis of petrochemical processes", Ph.D. thesis
PEC09-47	Ravendra Singh, 2009, "Model-based Computer-aided Framework for Design of Process Monitoring and Analysis Systems", Ph.D. thesis
PEC09-62	Ana Isabel Cerqueira de Sousa Gouveia Carvalho, 2009, "Design of Sustainable Chemical Processes: Systematic Retrofit Analysis Generation and Evaluation of Alternatives", Visiting Ph.D. student, Ph.D. thesis
PEC09-70	Rafiqul Gani, Ana Carvalho and Henrique A. Matos, 2009, "Process Design for CO2 and energy reduction", in "Managing CO2 Emissions", Hans-Joachim Leimkuehler (Editor), Wiley-Vch, Germany
PEC09-77	Meyer, A.S.;, Woodley, J.M.; and Gani, R.; 2009; "Process design and production of chemicals. Food ingredients, fuels and pharmaceuticals", in Engineering Challenges – Energy, Climate Change and Health, (Ed. C.B.Hansen), Technical University of Denmark, Lyngby, pp. 170-179
PEC10-02	Rafiqul Gani, Vipasha Soni, Piotr T. Mitkowski, **2010**, "Computer aided model based design and analysis of hybrid membrane reaction-separation systems", in "Comprehensive Membrane Science and Engineering", E. Drioli (Editor), Elsevier, The Netherlands
PEC10-13	Merlin Alvarado Morales, **2010**, "Process-product synthesis, design and analysis through the Group Contribution (GC) approach", Ph.D. thesis
PEC10-23 Book chp.	Gunnar Jonsson and Francesca Macedonia, 2010, "Fundamentals in reverse osmosis", In "Comprehensive Membrane Science and Engineering", E. Drioli (Editor), Elsevier, The Netherlands, Vol. 2, pp. 1-21

	B - Reviewed publications in International Journals
PEC07-51	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen and Sten Bay Jørgensen, 2009, "Improving Convergence of Iterative Feedback Tuning", Journal of Process Control, 19(4), pp. 570-578

PEC08-05	Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, 2009, "Model-based computer-aided framework for design of process monitoring and analysis systems", Computers and Chemical Engineering Journal, 33(1), pp. 22-42
PEC08-08	Ellegaard M.D., O'Connell J.P., Abildskov J., 2009, "Method for Predicting Solubilities of Solids in Mixed Solvents", AIChE Journal, 55(5), p. 1256-1264
PEC08-09	Piotr T. Mitkowski, Carsten Buchaly, Peter Kreis, Gunnar Jonsson, Andrzej Gorak, Rafiqul Gani, 2009, "Computer aided design, analysis and experimental investigation of membrane assisted batch reaction-separation systems", Computers and Chemical Engineering, 33(3), pp. 551-574
PEC08-10	Vipasha Soni, Jens Abildskov, Gunnar Jonsson, Rafiqul Gani, 2009, "A general model for membrane-based separation processes", Computers and Chemical Engineering, 33(3), pp. 644-659
PEC08-12	Kavitha C. Satyanarayana, Rafiqul Gani, Jens Abildskov, 2009, "Computer-aided polymer design using group contribution plus property models", Computers and Chemical Engineering, 33(5), pp. 1004-1013
PEC08-29	Søren Prip Beier, Gunnar Jonsson, 2009, "Critical flux determination by flux-stepping", AIChE Journal, doi: 10.1002/aic.12099
PEC08-30	Søren Prip Beier, Gunnar Jonsson, 2009, "A vibrating membrane bioreactor (VMBR): Macromolecular transmission – influence of extracellular polymeric substances", Chemical Engineering Science, 64(7), pp. 1436-1444
PEC08-32	Roberta Ceriani, Antonio J.A. Meirelles, Rafiqul Gani, **2010**, "Simulation of thin-film deodorizers in palm oil refining", Journal of Food Process Engineering, 33, pp. 208-225
PEC08-33	M Alvarado-Morales, J Terra, K V Gerneay, J M Woodley, R Gani, 2009, "Biorefining: Computer aided tools for sustainable design and analysis of bioethanol production", Chemical Engineering Research and Design, 87(9), pp. 1171-1183
PEC09-02	Netta Liin Rossing, Morten Lind, Niels Jensen and Sten Bay Jørgensen, **2010**, "A Functional HAZOP Methodology", Computers and Chemical Engineering, 34, pp. 244–253
PEC09-07	Jiang T, Sin G, Spanjers H, Nopens I, Kennedy MD, van der Meer W, Futselaar H, Amy G and Vanrolleghem PA, 2009, "Comparison of the modeling approach between membrane bioreactor and conventional activated sludge processes", Water Environment Research, 81(4), pp. 432-440
PEC09-08	Xavier Flores-Alsina, Ignasi Rodriguez-Roda, Gürkan Sin and Krist V. Gernaey, 2009, "Uncertainty and Sensitivity Analysis of Control Strategies using the Benchmark Simulation Model No1 (BSM1)", Water Science & Technology, 59(3), pp. 491-499
PEC09-09	John P. O'Connell, Rafiqul Gani, Paul M. Mathias, Gerd Maurer, James D. Olson, and Peter A. Crafts, 2009, "Thermodynamic Property Modeling for Chemical Process and Product Engineering: Some Perspectives", Industrial and Engineering Chemistry Research, 48(10), pp. 4619-4637
PEC09-11	Krist V. Gernaey, John M. Woodley and Gürkan Sin, 2009, "Introducing mechanistic models in Process Analytical Technology Education", Biotechnology Journal, Volume 4(5), pp. 593-598
PEC09-12	Gürkan Sin, Krist V. Gernaey, Marc B. Neumann, Mark C.M. van Loosdrecht and Willi Gujer, 2009, "Uncertainty analysis in WWTP model applications: a critical discussion using an example from design", Water Research, 43(11), pp. 2894-2906
PEC09-18	Georgios M. Kontogeorgis, Michael L. Michelsen, and Karsten H. Clement, 2009, "Teaching chemical engineering thermodynamics at three levels", Chemical Engineering Education, pp. 70-71

PEC09-21	Bao Lin, Bodil Recke, Torben M. Schmidt, Jørgen K.H. Knudsen, Sten Bay Jørgensen, 2009, "Data-driven soft sensor design with multiple-rate sampled data: a comparative study", Industrial & Engineering Chemistry Research, 48(11), pp. 5379-5387
PEC09-23	Roberta Ceriani, Rafiqul Gani, A.J.A. Meirelles, 2009, "Prediction of heat capacities and heats of vaporization of organic liquids by group contribution methods", Fluid Phase Equilibria, 283(1-2), pp. 49-55
PEC09-30	Gürkan Sin, Krist V. Gernaey and John M. Woodley, 2009, "Application of modeling and simulation tools for the evaluation of biocatalytic processes: a future perspective", Biotechnology Progress, 25, pp. 1529-1538
PEC09-31	M.V. Ruano, J. Ribes, Gürkan Sin, A. Seco and J. Ferrer, **2010**, "A systematic approach for fine-tuning of fuzzy controllers applied to WWTPs", Environmental Modelling and Software, 25, pp. 670-676
PEC09-33	Abildskov J., Ellegaard M.D., O'Connell J.P., 2009, "Correlation of Phase Equilibria and Liquid Densities for Gases with Ionic Liquids", Fluid Phase Equilibria, 286(1), pp. 85-96
PEC09-39	Gani, R., Gonzalez, H.E., 2009, "Analysis of a Concept for Predicting Missing Group Interaction Parameters of the UNIFAC Model Using Connectivity Indices", AIChE Journal, 55(6), pp. 1626-1627
PEC09-49	Jose Seoane, Gürkan Sin, Laurent Lardon, Krist V. Gernaey, Barth F. Smets, **2010**, "A new extant respirometric assay to estimate intrinsic growth parameters applied to study plasmid metabolic burden", Biotechnology and Bioengineering, 105, pp. 141–149
PEC09-50	Belia E., Amerlinck Y., Benedetti L., Johnson B., Sin G., Vanrolleghem P.A., Gernaey K.V., Gillot S., Neumann M. B., Rieger L., Shaw A. and Villez K., 2009, "Wastewater treatment modelling: dealing with uncertainties", Water Science and Technology, 60(8), pp. 1929-1941
PEC09-51	Sin, G.; Eliasson Lantz, A.; and Gernaey, K.V.; 2009, "Good modelling practice (GMoP) for PAT applications: Propagation of input uncertainty and sensitivity analysis", Biotechnology Progress, 25, pp. 1043-1053
PEC09-53	Mohd Kamaruddin Abd Hamid; Gurkan Sin; Rafiqul Gani, **2010**, "Integration of process design and controller design for chemical processes using model-based methodology", Computers and Chemical Engineering, 34(5), pp. 683-699
PEC09-55	Naveed Ramzan, Muhammad Faheem, Rafiqul Gani, Werner Witt, **2010**, "Multiple Steady States Detection in a Packed-Bed Reactive Distillation Column using Bifurcation Analysis", Computers & Chemical Engineering,34(4), pp. 460-466
PEC09-68	Veronique van Speybroeck, Rafiqul Gani and Robert Johan Meier, **2010**, "The calculation of thermodynamic properties of molecules", Chemical Society Review, 39, pp. 1764-1779
PEC09-78	Manuel Pinelo, Gunnar Jonsson, Anne S. Meyer, 2009, "Membrane technology for purification of enzymatically produced oligosaccharides: Molecular and operational features affecting performance", Separation and Purification Technology, 70, pp. 1-11
PEC10-10	R. Ganigué, E.I.P. Volcke, S. Puig, M.D. Balaguer, J. Colprim and G. Sin, **2010**, "Systematic model development for partial nitrification of landfill leachate in a SBR", Biotechnology and Bioengineering, 61(9), pp. 2199-2210
PROCESS	Cervera, A.E., Petersen, N., Eliasson Lantz, A., Larsen, A., Gernaey, K.V., 2009, "Application of near-infrared spectroscopy for monitoring and control of cell culture and fermentation", Biotechnol. Prog., 25, pp. 1561-1581
PROCESS	Petersen, N., Ödman, P., Cervera Padrell, A.E., Stocks, S., Eliasson Lantz, A., Gernaey K.V., **2010**, "In situ near infrared spectroscopy for analyte-specific monitoring of glucose and ammonium in Streptomyces coelicolor fermentations", Biotechnol. Prog., 26, pp. 263-271

PROCESS	Boisen, A., Christiansen, T.B., Fu, W., Gorbanev, Y.Y., Hansen, T.S., Jensen, J.S., Klitgaard, S.K., Pedersen, S., Riisager, A., Ståhlberg, T., and Woodley, J.M., 2009, "Process integration for the conversion of glucose to 2,5-furandicarboxylic acid", ChERD, 87, pp. 1318-1327
PEC10-15	A.Carvalho, H.A. Matos, R. Gani, 2009, "Design of batch operations: Systematic methodology for generation and analysis of sustainable alternatives", Computers and Chemical Engineering, 33(12), pp. 2075-2090
PROCESS	Schäpper D., Muhd Nazrul Hisham Zainal Alam, Szita N., Eliasson Lantz A and Gernaey K.V. (2009) Application of microbioreactors in fermentation process development: a review. Analytical and Bioanalytical Chemistry, 395, 679-695.
PROCESS	Flores-Alsina X., Comas J., Rodriguez-Roda I., Gernaey K.V. and Rosen C. (2009) Including the effects of filamentous bulking sludge during the simulation of wastewater treatment plants using a risk assessment model. Water Research, 43, 4527-4538.
PROCESS	Flores-Alsina X., Comas J., Rodríguez Roda I., Poch M., Gernaey K.V. and Jeppsson U. (2009) Evaluation of plant-wide WWTP control strategies including the effects of filamentous bulking sludge. Water Science and Technology, 60(8), 2093-2103.
PROCESS	Ödman P., Lindvald Johansen C., Olsson L., Gernaey K.V. and Eliasson Lantz A. (2009) On-line estimation of biomass, glucose and ethanol in *Saccharomyces cerevisiae* cultivations using in-situ multi-wavelength fluorescence and software sensors. Journal of Biotechnology, 144, 102-112.
PROCESS	Petersen N., Ödman P., Cervera Padrell A.E., Stocks S., Eliasson Lantz A. and Gernaey K.V. (2010) In situ near infrared spectroscopy for analyte-specific monitoring of glucose and ammonium in *Streptomyces coelicolor* fermentations. Biotechnology Progress, 26, 263-271.
PROCESS	Corominas Ll., Rieger L., Takács I., Ekama G., Hauduc H., Vanrolleghem P.A., Oehmen A., Gernaey K.V., van Loosdrecht M.C.M. and Comeau Y. (2010) New framework for standardized notation in wastewater treatment modelling. Water Science and Technology, 61, 841-857.
PROCESS	Bracewell D., Gernaey K.V., Glassey J., Hass V.C., Heinzle E., Mandenius C.-F., Olsson I.-M., Racher A., Staby A., Titchener-Hooker N. (2010) Report and recommendation of a workshop on education and training for measurement, monitoring, modelling & control (M3C) in biochemical engineering. Biotechnology Journal, 5, 359-367.
PROCESS	Zainal Alam M.N.H., Schäpper D. and Gernaey K.V. (2010) Embedded resistance wire as heating element for temperature control in microbioreactors. Journal of Micromechanics and Microengineering, 20, 055014. (doi: 10.1088/0960-1317/20/5/055014)
PROCESS	Ödman P., Lindvald Johansen C., Olsson L., Gernaey K.V. and Eliasson Lantz A. (2010) Sensor combination and chemometric variable selection for on-line monitoring of *Streptomyces coelicolor* fed-batch cultivations. Applied Microbiology and Biotechnology, 86, 1745-1759.
PROCESS	CHEN BH, MICHELETTI M, BAGANZ F, WOODLEY JM, LYE GJ. 2009. An efficient approach to bioconversion kinetic model generation based on automated microscale experimentation integrated with model driven experimental design. Chem Eng Sci. 64, 403-409.
PROCESS	LEAK DJ, SHELDON RA, WOODLEY JM, ADLERCREUTZ P. 2009. Biocatalysts for selective introduction of oxygen. Biocat. Biotrans. 27, 1-26.
PROCESS	SHITU JO, CHARTRAIN M, WOODLEY JM. 2009. Evaluating the impact of substrate and product concentration on a whole-cell biocatalyst during a Baeyer-Villiger reaction. Biocat Biotrans. 27(2), 107-117.
PROCESS	SHITU JO, WOODLEY JM, WNEK R, CHARTRAIN M, HEWITT CJ. 2009. Induction studies with Escherichia coli expressing recombinant interleukin-13 using multi-paramater flow cytometry. Biotechnol. Lett. 31, 577-584.

PROCESS	WONG M, WRIGHT M, WOODLEY JM, LYE GJ. 2009. Enhanced recombinant protein synthesis in batch and fed-batch Escherichia coli fermentation based on removal of inhibitory acetate by electrodialysis. J Chem Tech Biotechnol. 84(9), 1284-1291.
PROCESS	GORBANEV YY, KLITGAARD SK, WOODLEY JM, RIISAGER A. 2009. Gold catalyzed aerobic oxidation of 5-hydroxymethylfurfural in water at ambient temperature. ChemSusChem. 2, 672-675.
PROCESS	SAYAR NA, CHEN BH, LYE GJ, WOODLEY JM. 2009. Modelling and simulation application to a transketolase mediated reaction; sensitivity analysis of kinetic parameters. Biochem Eng J. 47, 1-9.
PROCESS	SAYAR NA, CHEN BH, LYE GJ, WOODLEY JM. 2009. Process modelling and simulation of a transketolase mediated reaction; analysis of alternative modes of operation. Biochem Eng J. 47, 10-18.
PROCESS	HANSEN TH, WOODLEY JM and RIISAGER A. 2009. Efficient microwave-assisted synthesis of 5-hydroxymethylfurfural from concentrated aqueous fructose. Carbohydrate Research. 344, 2568-2572.
PROCESS	SMITH MEB, CHEN BH, HIBBERT EG, KAULMANN U, SMITHIES K, GALMAN J, BAGANZ F, DALBY PA, HAILES HC, LYE GJ, WARD JM, WOODLEY JM, MICHELETTI M. **2010**. Biocatalytic synthesis of Chiral Amino Alcohols: A Concise Transketolase / Transaminase - Mediated Synthesis of (2S, 3S)-2-Aminopentane-1,3-diol. Org.Proc Res Dev. 14, 99-107.
PROCESS	P.N.R. Vennerstrøm, C.H. Christensen, S. Pedersen, J.-D. Grunwaldt, J.M. Woodley, **2010**, "Next-generation catalysis for renewables: Combining enzymatic with inorganic heterogeneous catalysis for bulk chemical production", ChemlatChem, 1, pp. 249-258
PROCESS	Tufvesson, P., Fu, W., Jensen, J.S., and Woodley, J.M., **2010**, "Process considerations for the scale-up and implementation of biocatalysis", Food and Bioproducts Processing, 88, pp. 3-11

	C - In press/Submitted Manuscripts
PEC08-11	Ricardo Morales-Rodriguez, Rafiqul Gani, 2008, "A systematic model-based framework for chemical product-process development", Computers and Chemical Engineering, Submitted
PEC08-28	Piotr Szewczykowski, Gunnar Jonsson, Rolf H. Berg, Martin E. Vigild, Sokol Ndoni, 2008, "Gyroid membranes made from nanoporous block copolymers", Journal of Membrane Science, Submitted
PEC09-06	R. Singh, K.V. Gernaey, R. Gani, **2010**, "ICAS-PAT: A Software for Design, Analysis & Validation of PAT Systems", Computers & Chemical Engineering, Accepted (in Press), doi:10.1016/j.compchemeng.2009.06.021
PEC09-10	Kavitha C. Satyanarayana, Jens Abildskov, Rafiqul Gani, Georgia Tsolou, Vlasis G. Mavrantzas, 2009, "Computer aided polymer design using multiscale modeling", Brazilian Journal of Chemical Engineering, Accepted (In Press)
PEC09-34	Romain Privat, Jean-Nöel Jaubert, Rafiqul Gani, 2009, "PC-SAFT equation of state: easy determination of model parameters and their use for prediction of pure component and mixture properties", AIChE Journal, Submitted
PEC09-37	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, John Bagterp Jørgensen, **2010**, "ARX-Model based Model Predictive Control with Offset-Free Tracking", 20th European Symposium on Computer Aided Process Engineering - ESCAPE20, Accepted (In Press)

PEC09-38	Ricardo Morales-Rodriguez, Marie Capron, Jakob Kjøbsted Huusom and Gürkan Sin, **2010**, ”Controlled fed-batch operation for enzymatic cellulose hydrolysis in 2G bioethanol production”, 20th European Symposium on Computer Aided Process Engineering - ESCAPE20, Accepted (In Press)
PEC09-42	Jakob Kjøbsted Huusom, Håkan Hjalmarsson , Niels Kjølstad Poulsen, Sten Bay Jørgensen, 2009,” A Design Algorithm using External Perturbation to Improve Iterative Feedback Tuning Convergence”, Automatica, Submitted
PEC09-48	Gürkan Sin, Anne S. Meyer and Krist V. Gernaey , 2009, “Assessing Reliability of Cellulose Hydrolysis Models to Support Biofuel Process Design – Identifiability and Uncertainty Analysis”, Computers and Chemical Engineering, Submitted
PEC09-52	Oscar Andres Prado-Rubio, Martin Møllerhøj, Sten B. Jørgensen, Gunnar E. Jonsson, **2010**, ”Modeling Donnan Dialysis Separation for Carboxylic Anion Recovery”, Computers and Chemical Engineering (ESCAPE 19 – special issue), Accepted/in Press, doi: 10.1016/j.compchemeng.2010.03.003
PEC09-54	Rasmus Wedberg, John P. O’Connell, Günther H. Peters, Jens Abildskov, 2009, “Accurate Kirkwood-Buff integrals from molecular simulations”, Molecular Simulation, Accepted
PEC09-56	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, **2010**, ”Tuning of Methods for Offset Free MPC based on ARX Model Representations”, Proceedings of the American Control Conference (ACC), Accepted
PEC09-58	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, 2009, ”Offset-Free Model Predictive Control Based on ARX Models”, Journal of Process Control, Submitted
PEC09-59	Oscar Andres Prado-Rubio, Sten Bay Jørgensen and Gunnar Jonsson, **2010**, ”Control System Development for Integrated Bioreactor and Membrane Separation Process”, 20th European Symposium on Computer Aided Process Engineering - ESCAPE20, Accepted (In Press)
PEC09-60	Oscar Andres Prado-Rubio, John Bagterp Jørgensen and Sten Bay Jørgensen, **2010**, ”Systematic Model Analysis for Single Cell Protein (SCP) Production in a U-Loop Reactor”, 20th European Symposium on Computer Aided Process Engineering - ESCAPE20, Accepted (In Press)
PEC09-61	Gernaey, K.V.; Eliasson, Lantz A.; Woodley, J.; and Sin, G.; 2009, “Application of mechanistic models to fermentation and biocatalysis”, Trends in Biotechnology, Submitted
PEC09-63	Merlin Alvarado-Morales, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, **2010**, “Synthesis, Design and Analysis of Downstream Separation in Bio-refinery Processes through a Group-Contribution Approach”, 20th European Symposium on Computer Aided Process Engineering - ESCAPE20, Accepted (In Press)
PEC09-64	Philip Lutze, Alicia Román-Martinez, John M. Woodley, Rafiqul Gani, **2010**, “A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes”, 20th European Symposium on Computer Aided Process Engineering - ESCAPE20, Accepted (In Press)
PEC09-65	Carlos A. Diaz-Tovar, Roberta Ceriani, Rafiqul Gani and Bent Sarup, 2009, “Systematic methodology and property prediction of fatty systems for process design/analysis in the oil and fat industry**”,** Brazilian Journal of Chemical Engineering, Submitted
PEC09-66	Merlin Alvarado–Morales, Mohd. Kamaruddin Abd Hamid, Gürkan Sin, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2009, “A Model-Based Methodology for Simultaneous Design and Control of a Bioethanol Production Process”, Computers and Chemical Engineering Journal, Submitted

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PEC10-25	Rafiqul Gani, **2010**, "CAPEC Research Report 2010", CAPEC Internal Report, DTU-KT, Lyngby, Denmark

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F	Jamal Rashed and Rafiqul Gani, 2009, "Model-based retrofit design and analysis of petrochemical processes", 1st Annual Gas Processing Symposium, Doha, Qatar, 10-12 January
F	Sten Bay Jørgensen, 2009, "Modelling for Process and Control Design", Nordic Process Control Workshop '09, NPCW09, Porsgrunn, Norway, 29-30 January
F	Oscar Andres Prado Rubio, Sten Bay Jørgensen, Gunnar Jonsson, 2009, "Modeling Reverse Electro-Enhanced Dialysis for Integration with Lactic Acid Fermentation", Nordic Process Control Workshop '09, NPCW09, Porsgrunn, Norway, 29-30 January
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F	Sten Bay Jørgensen, 2009, "Modelling Paradigms for Process Design, Identification and Control", MIC´09: Modelling, Identification and Control, IASTED conference, Innsbruck, Austria, 16-18 February **(Invited Keynote Lecture)**
F	R. Singh, K. V. Gernaey, R. Gani, 2009, "ICAS-PAT: A new software tool for systematic design/validation of process monitoring and analysis systems (PAT systems)", APACT-09, Glasgow, UK, 5-7 May
	AMIDIQ, Mazatlan, Mexico, 19-22 May – 4 presentations
F	Rafiqul Gani, 2009, "Managing the complexity in product-process design", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May **(Plenary Lecture)**
F	Carlos A. Diaz-Tovar, Roberta Ceriani, Rafiqul Gani and Bent Sarup, 2009, "Simulation and Optimization of a Solvent Recovery Process in the Vegetable Oil Industry", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May

F	Alicia Román Martínez, Rafiqul Gani, John M. Woodley, 2009, "Design methodology for intensified bioprocesses", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May
F	Ricardo Morales-Rodríguez, Rafiqul Gani, 2009, "Product-Process Design Multiscale Modelling Framework", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May
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F (poster)	Linfeng Yuan, Lars Korsholm, Sune Jakobsen, John Woodley, Gunnar Jonsson, 2009, "Study of Electro-membrane Filtration in Enzyme Fractionation using Amino Acid", PERMEA2009, Prague, Czech Republic, 7-11 June
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F (poster)	Mohd Kamaruddin Abd Hamid, Gurkan Sin, Rafiqul Gani, 2009, "Determination of optimal design and control decisions for reactor-separator systems with recycle", Foundations of Computer-Aided Process Design (FOCAPD) 2009, Breckenridge, Colorado, June 7 – 12
F	Gürkan Sin, Anne S Meyer, Krist V. Gernaey, 2009, "Are Mechanistic Cellulose-Hydrolysis Models Reliable for Use in Biofuel Process Design? – Identifiability and Sensitivity Analysis", Foundations of Computer-Aided Process Design (FOCAPD) 2009, Breckenridge, Colorado, June 7 – 12
F (poster)	Ana Carvalho, Henrique A. Matos, Rafiqul Gani, 2009, "Analysis and generation of sustainable alternatives: Continous and batch processes using SustainPro", Foundations of Computer-Aided Process Design (FOCAPD) 2009, Breckenridge, Colorado, June 7 – 12
F	Arunprakash T. Karunanithi, Rafiqul Gani, Luke E.K. Achenie, 2009, "Biodiesel Process Design through a Computer-aided Molecular Design Approach", Foundations of Computer-Aided Process Design (FOCAPD) 2009, Breckenridge, Colorado, June 7 – 12
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F	Ricardo Morales-Rodríguez, Rafiqul Gani, 2009, "Multiscale Modelling Framework for Chemical Product-Process Design", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14-17 June
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F (poster)	Netta Liin Rossing, Morten Lind, Niels Jensen and Sten Bay Jørgensen, 2009, "A Goal Based HAZOP Assistant", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14-17 June
F (poster)	Jamal Rashed, Rafiqul Gani, 2009, "Model-based retrofit design and analysis of petrochemical processes", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14-17 June
F	Pimporn Lek-utaiwan, Bunyaphat Suphanit, Nakarin Mongkolsiri, Rafiqul Gani, 2009, "Integrated design of solvent based extractive separation processes including experimental validation", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14-17 June
	17th Symposium on Thermophysical Properties, Boulder, CO, USA, 21-26 June – 1 presentation
F	Martin Ellegaard, Jens Abildskov, John O'Connell, 2009, "Densities and isothermal compressibilities of ionic liquids: Data retrieval, modelling, and application", Seventeenth Symposium on Thermophysical Properties, Boulder, CO, USA, 21-26 June
F	Jens Abildskov, Martin Ellegaard, John O'Connell, 2009, "Solubilities, Henry's law constants, and direct correlation function integrals of gases in ionic liquids", Seventeenth Symposium on Thermophysical Properties, Boulder, CO, USA, 21-26 June
F	Martin Ellegaard, Jens Abildskov, John O'Connell, 2009, "Solubility of solids in mixed solvents: modeling and data reduction", Seventeenth Symposium on Thermophysical Properties, Boulder, CO, USA, 21-26 June
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F	Romain Privat, Rafiqul Gani and Jean-Noël Jaubert, 2009, "Prediction of thermodynamic properties of pure components and mixtures: cubic equations of state versus molecular theory-derived equations of state: a short comparison", JETC10, Copenhagen, DK, 22-24 June
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F	Martin Ellegaard, John O'Connell, Jens Abildskov, 2009, "Corresponding states correlation for liquids densities and gas solubilities in ionic liquids", 24th European Symposium on Applied Thermodynamics, ESAT-2009, Santiato de Compostela, Spain, 27 June – 1 July
F	Romain Privat, Rafiqul Gani and Jean-Noël Jaubert, 2009, "Application of the GC-plus approach to PC-SAFT EOS and prediction of phase Equilibria", 24th European Symposium on Applied Thermodynamics, ESAT-2009, Santiato de Compostela, Spain, 27 June – 1 July
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F (poster)	Alicia Román Martinez, Rafiqul Gani, John M. Woodley, 2009, "Design Strategies for Neuraminic Acid Synthesis: Comparative Study of Chemical and Biochemical Routes and Integration of Purification Steps", Biotrans 2009, Berne, Switzerland, 5-9 July

F (poster)	Chutima Swangkotchakorn, Rafiqul Gani, John M. Woodley, Jan-Dierk Grunwaldt, 2009, "Optimization of tailor-made chemicals from renewable and non-renewable sources", Biotrans 2009, Berne, Switzerland, 5-9 July
F (poster)	Santacoloma, P.A.; Sin, G.; Gernaey, K.V.; Woodley, J.M.; 2009, "Systematic framework for modeling multi-enzymatic synthetic processes", Biotrans 2009, Bern, Switzerland, 5-9 July
F PROCESS	Fu, W., Jensen, J. S., Christensen, T., Boisen, A., Pedersen, S., Riisager, A., Woodley, J., 2009, "Process Design of Chemo-enzymatic Synthetic Cascades", Biotrans 2009, Bern, Switzerland, 5-9 July
	FOMMS, Seattle, USA, 12-16 July –1 presentation
F	Rasmus Wedberg, John P. O'Connell, Günther H. Peters, Jens Abildskov, 2009, "Accurate Kirkwood-Buff integrals from molecular dynamics simulations", FOMMS, Blaine, WA, USA, 12-16 July
	1st International Congress on Sustainability Science & Engineering (ICOSSE-2009), Cincinnati, USA, 10-12 August
F	Rafiqul Gani and John Woodley 2009, "Sustainable Design of Chemical and Biochemical Processes: The Role of Models and Modeling", 1st International Congress of Sustainability Science and Engineering (ICOSSE-2009), Cincinnati, OH, USA, 10-12 August **(Invited Keynote Lecture)**
	PSE-2009, Salvador Bahia, Brazil, 16-20 August – 9 presentations + 1 Plenary Lecture
F	Carlos A. Diaz-Tovar, Roberta Ceriani, Rafiqul Gani and Bent Sarup, 2009, "Systematic Representation and Property Prediction of Fatty Systems for Process Design/Analysis in the Oil and Fat Industry", 10th International Symposium on Process System Engineering, PSE2009, Salvador de Bahia, Brazil, 16-20 August
F (poster)	Jakob K. Huusom, Niels K. Poulsen, Sten Bay Jørgensen, 2009, "Iterative Feedback Tuning of State Space Control Loops with Observers Given Model Uncertainty", 10th International Symposium on Process System Engineering, PSE2009, Salvador de Bahia, Brazil, 16-20 August
F	Elisa Conte, Ricardo Morales-Rodriguez, Rafiqul Gani, 2009, "The Virtual Product-Process Design Laboratory for the Design and Analysis of Formulations", 10th International Symposium on Process Systems Engineering, PSE2009, Salvador de Bahia, Brazil, 16-20 August
F (poster)	Oscar Andres Prado-Rubio, Sten Bay Jørgensen, Gunnar Jonsson, 2009, "Tool for Optimizing the Design and Operation of Reverse Electro-Enhanced Dialysis of Monoprotic Carboxylic Acids", 10th International Symposium on Process System Engineering, PSE2009, Salvador de Bahia, Brazil, 16-20 August
F	Rafiqul Gani, 2009, "Modelling for PSE and Product-Process Design", 10th International Symposium on Process Systems Engineering, PSE2009, Salvador de Bahia, Brazil, 16-20 August **(Plenary Lecture)**
F	Gürkan Sin, Anna Eliasson Lantz, Krist V. Gernaey, 2009, "Sensitivity Analysis of Non-Linear Dynamic Models: Prioritizing Experimental Research", 10th International Symposium on Process Systems Engineering, PSE2009, Salvador do Bahia, Brazil, 16–20 August
F	Merlin Alvarado-Morales, Mohd Kamaruddin Abd Hamid, Gurkan Sin, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2009, "A Model-Based Methodology for Simultaneous Design and Control of a Bioethanol Production Process", 10th International Symposium on Process Systems Engineering, PSE2009, Salvador do Bahia, Brazil, 16–20 August

F	Ana Carvalho, Henrique A. Matos, Rafiqul Gani, 2009, "Sustainability Analysis of Chemical Processes Plants Using a Hybrid Heuristic and Indicator Model", 10th International Symposium on Process Systems Engineering, PSE2009, Salvador do Bahia, Brazil, 16–20 August
F	Kavitha Chelakara Satyanarayana, Jens Abildskov, Rafiqul Gani, Georgia Tsolou, Vlasis G. Mavrantzas, 2009, "Multiscale Modelling for Computer Aided Polymer Design", 10th International Symposium on Process Systems Engineering , PSE2009, Salvador do Bahia, Brazil, 16–20 August
F	Edelmira D. Gálvez, Luis A. Cisternas, Gonzalo Herrera, and Rafiqul Gani, **2009**, "A Group Contribution Method for Mineral Flotation Circuit Design", 10th International Symposium on Process Systems Engineering, PSE2009, Salvador do Bahia, Brazil, 16–20 August
	10th European Control Conference – ECC09, Budapest, Hungary, 23-26 August – 1 presentation
F	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen and Sten Bay Jørgensen, 2009, "Data Driven Tuning of State Space Controllers with Observes", 10th European Control Conference – ECC09, Budapest, Hungary, 23-26 August
	WCCE8, Montreal, Canada, 23-27 August – 1 presentation
F	Krist V. Gernaey, Ravendra Singh and Rafiqul Gani, 2009, "A systematic computer aided framework for design and analysis of PAT system", World Congress of Chemical Engineering, WCCE8, Montreal, Canada, 23-27 August
	12th Nordic Filtration Symposium, Gothenburg, Sweden, 26-27 August – 1 Keynote Lecture
F	Gunnar Jonsson, 2009, "Using membrane techniques with aspects on energy and environment", 12th Nordic Filtration Symposium, Gothenburg, Sweden, 26-27 August **(Keynote Lecture)**
	Euromembrane 2009, Montpellier, France, September 6-10 – 2 presentations
F	Gunnar Jonsson, 2009, "Modelling aroma stripping under various forms of membrane distillation processes", Euromembrane 2009, Montpellier, France, September 6-10
F (poster)	J. Benavente, V. Silva, P. Prádanos, L. Palacio, A. Hernánez, G. Jonsson, 2009, "Contributions to the electric potential appearing when a pressure drop is applied through a nanofiltration membrane", Euromembrane 2009, Montpellier, France, September 6-10
	2nd IWA Specialized Conference on nutrient management in wastewater treatment, Krakow, Poland, 6-9 September – 1 presentation
F	Ganigué R., Volcke E.I.P., Puig S., Balaguer M.D., Colprim J. and Sin G., 2009, "Systematic model development for partial nitrification of landfill leachate in a SBR", 2nd IWA Specialized Conference on nutrient management in wastewater treatment, Krakow, Poland, 6-9 September
	ECB 14, Barcelona, Spain, 13-16 September – 2 presentations
F (poster)	Gernaey, K.V.; Woodley, J.M.; Eliasson Lantz, A.; and Sin, G.; 2009, "Mechanistic models and advanced model analysis within a PAT framework", 14th European Congress on Biotechnology (ECB 14), Barcelona, Spain, 13-16 September
F (poster) PROCESS	Petersen, N., Ödman, P., Cervera Padrell, A.E., Eliasson Lantz, A., Stocks, S., Gernaey K., 2009, "Monitoring of *S. coelicolor* fermentations using in-situ NIR", 14th European Congress on Biotechnology (ECB14), Barcelona, Spain, 13-16 September
	Thermodynamics 2009, London, UK, 23-25 September – 1 presentation

F	Martin Ellegaard, Jens Abildskov, John O'Connell, 2009, "Thermodynamic properties and gas solubilities in ionic liquids from a group contribution approach to fluctuation solution theory", Thermodynamics 2009, London, UK, 23-25 September
	5th Dubrovnik conference on sustainable Development of Energy Water and Environment Systems, Dubrovnik, Croatia, 29 September-3 October –1 Keynote presentation
F	Gürkan Sin, 2009, "Multi-criteria decision making under uncertainty: Energy efficient and low-carbon wastewater treatment", 5th Dubrovnik conference on sustainable Development of Energy Water and Environment Systems, Dubrovnik, Croatia, 29 September – 3 October **(Keynote Lecture)**
	NPS-9, 26-28 October – 1 Keynote Presentation
F	Rafiqul Gani, 2009, "Sustainable product centric process design", Netherlands Process Technology Symposium 2009 (NPS-9), Veldhoven, The Netherlands, 26-28 October **(Keynote Lecture)**
	AIChE, 8-13 November 2009 – 13 presentations + 3 posters
F	Rasmus Wedberg, John P. O'Connell, Günther Peters and Jens Abildskov, 2009, "Accurate Kirkwood-Buff Integrals From Molecular Dynamics Simulations", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November
F	Alicia Román Martínez, Rafiqul Gani and John M. Woodley, 2009, "A Systems Approach for Design of Intensified Bio-Pharmaceutical Processes", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November
F	Merlín Alvarado-Morales, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2009, "Synthesis, Design and Analysis of Downstream Separation in Chemical and Bio-Processes", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November
F	Albert E. Cervera, Tommy Skovby, Søren Kiil, Rafiqul Gani and Krist V. Gernaey, 2009, "Moving From Batch towards Continuous Organic-Chemical Pharmaceutical Production", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November
F	Dres Foged Olsen, John Bagterp Jorgensen, John Villadsen, Gürkan Sin and Sten Bay Jorgensen, 2009, "Modelling, Simulation and Optimization of Single-Cell Protein Production in a U-Loop Reactor", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
F	Chutima Swangkotchakorn, Rafiqul Gani, John Woodley and Jan-Dierk Grunwaldt, 2009, "Sustainable Bioprocess Synthesis Routes for Tailor-Made Chemicals", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
F	Martina Heitzig, Gürkan Sin, Peter Glarborg and Rafiqul Gani, "A Computer-Aided Modelling Tool for Efficient Model Identification and Analysis", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
F	Ricardo Morales-Rodriguez, Gürkan Sin, Krist V. Gernaey, Anne S. Meyer, 2009, "Development of An Integrated Dynamic Model for Bioethanol Production From Lignocellulosic Biomass", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November
F	Philip Lutze, Rafiqul Gani and John M. Woodley, 2009, "A Systematic Methodology to Synthesize and Design Processes, Incorporating Process Intensification", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November
F	Elisa Conte, Rafiqul Gani, Ricardo Morales-Rodriguez, 2009, "The Virtual Product-Process Design Laboratory for the Design of Formulated Products", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November

F	Noor Asma Fazli Bin Abdul Samad, Ravendra Singh, Gürkan Sin, Krist V. Gernaey and Rafiqul Gani, 2009, "Application of ICASPAT On Design of Process Monitoring and Control System for a Batch Cooling Crystallization Process through Hybrid Multiscale Model-Based Analysis", AIChE Annual Meeting 2009, Nashville, TN, USA, 8-13 November
F	Martina Heitzig, Ricardo Morales-Rodriguez, Gürkan Sin, Peter Glarborg and Rafiqul Gani, 2009, "A Computer-Aided Tool for Applying the Multiscale Modeling Needs in Innovative Product-Process Engineering", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
F (poster)	Romain Privat, Rafiqul Gani and Jean-Noel Jaubert, 2009, "Direct Calculation of PC-SAFT Parameters From Experimental LVE Data and From a GC-Plus Approach", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
F (poster)	Santacoloma PA, Sin G, Gernaey KV, Woodley JM, 2009, "Sensitivity Analysis of a Two-Enzyme One-Pot System for Production of Lactobionic Acid", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
F PROCESS	Fu, W., Jensen, J. S., Boisen, A., Pedersen, S., Riisager, A., Woodley, J., 2009, "Process Design of Chemo-enzymatic Synthetic Cascades", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
F (poster) PROCESS	Fu, W., and Woodley, J., 2009, "Computer aided Process Design of Chemo-enzymatic Synthetic Cascades", AIChE Annual Meeting, Nashville, TN, USA, 8-13 November
	F - Conference Presentations 2010
F	Ana Carvalho, Rafiqul Gani and Henrique Matos , 2010, "Design of sustainable processes: Systematic generation and evaluation of alternatives", 2nd Annual Gas Processing Symposium 2010, Doha, Qatar, 11-14 January **(Best Paper Award)**
F	Rafiqul Gani, 2010, "Design challenges and sustainability issues in gas processing: A view from academia", 2nd Annual Gas Processing Symposium 2010, Doha, Qatar, 11-14 January **(Invited Lecture)**
F	Gürkan Sin, Anna Eliasson Lantz, Krist V. Gernaey, 2010, "Perspectives on the use of global uncertainty and sensitivity analysis methods in a PAT context", 24th International Foundation Process Analytical Chemistry (IFPAC®), Baltimore, Maryland, USA, 31 January – 4 February
F	Ravendra Singh, Noor Asma Fazli Abdul Samad, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2010, "Mechanistic modeling for systematic design and analysis of PAT systems", 24th International Foundation Process Analytical Chemistry (IFPAC®), Baltimore, Maryland, USA, 31 January - 4 February **(Invited Lecture)**
F (poster)	Carlos Axel Díaz-Tovar, Rafiqul Gani, Bent Sarup, 2010, "Towards the Merging of Property Prediction & Process Design/Analysis in the Edible Oil Industry", CAPE Forum 2010, Aachen, Germany, 11-12 March
F	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, John Bagterp Jørgensen, 2010, "Tuning of ARX-based Model Predictive Control for Offset-free Tracking", CAPE Forum, Aachen, Germany, 11-12 March
F	Mohd. Kamaruddin Abd. Hamid, Gurkan Sin, Rafiqul Gani, 2010, "Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problems for Reactor-Separator-Recycle Systems", CAPE Forum, Aachen, Germany, 11-12 March
F	Alicia Román-Martínez, Rafiqul Gani, John M. Woodley, 2010, "Model-based Design and Analysis of Integrated Biocatalytic Processes", CAPE Forum 2010, Aachen, Germany, 11-12 March

F	Rafiqul Gani, 2010, "Thermodynamics – our molecular sister or just a forgotten relative?", CAPE Forum 2010, Aachen, Germany, 11-12 March **(Invited Lecture)**
F	Gürkan Sin, M.V. Ruano, Marc B. Neumann, J. Ribes, Krist V. Gernaey, J. Ferrer , Mark C.M. van Loosdrecht and Willi Gujer, 2010, "Sensitivity analysis in the WWTP modelling community – new opportunities and applications", 2nd IWA/WEF Wastewater Treatment Modelling Seminar, Mont-Sainte-Anne, Quebec, Canada. March 26-31
F	Sascha Sansonetti, Stefano Curcio, Vincenza Calabrò, Gürkan Sin and Gabriele Iorio, 2010, "Feasibility of the batch fermentation process of Ricotta Cheese Whey (RCW)", IBIC2010, Padua, Italy, 11-14 April
F	Gürkan Sin, Anna Eliasson Lantz, Krist V. Gernaey, 2010, "Perspectives on the use of global uncertainty and sensitivity analysis methods in a PAT context", 24th International Foundation Process Analytical Chemistry (IFPAC®), Baltimore, Maryland, USA, 31 January – 4 February
F	Singh, R., Samad, N.A.F.A., Sin, G., Gernaey, K. V., Gani, R., 2010, "Systematic method and tool for design, analysis &/or validation of PAT systems", APACT-10, Manchester, UK, 28-30 April
F	Fu, W., Jensen, J. S., Boisen, A., Pedersen, S., Riisager, A., Gani, R., Woodley, J., 2010, "Process Design of Chemo-enzymatic Synthetic of 2,5-dicarbonoxylic acid", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May
F (poster)	N. Iyara, K. Siemanond, R. Gani, 2010, "Sustainable design for an olefin process", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May **(Best Poster Award)**
F (poster)	P. Tansutapanich, P. Malakul, R. Gani, 2010, "Sustainable process design for lignocellulosic-based bioethanol using life cycle assessment technique", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May
F	R. Gani, 2010, "Solvents, green chemistry and sustainable product-process design", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May **(Plenary Lecture)**
F	Ricardo Morales-Rodriguez, Krist V. Gernaey, Anne S. Meyer and Gürkan Sin, 2010, "Development of a mathematical model describing hydrolysis and co-fermentation of C6 and C5 sugars", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May
F (poster)	C.A. Diaz Tovar, R. Gani, B. Sarup, 2010, "Lipid technology: Property prediction and process design/analysis in the edible oil industry", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May
F (poster)	C. Aguirre, L. Cisternas, J. Continho, R. Gani, 2010, "Computer-aided design of ionic-liquids by group contribution methods", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May
F (poster)	A.A. Mustaffa, G.M. Kontogeorgis, R. Gani, 2010, "Analysis and application of GC plus models for property prediction of organic chemical systems", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May
F	Elisa Conte, Rafiqul Gani and Tahir I. Malik, 2010, "The Virtual Product-Process Design Laboratory to Manage the Complexity in Formulation Design", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May

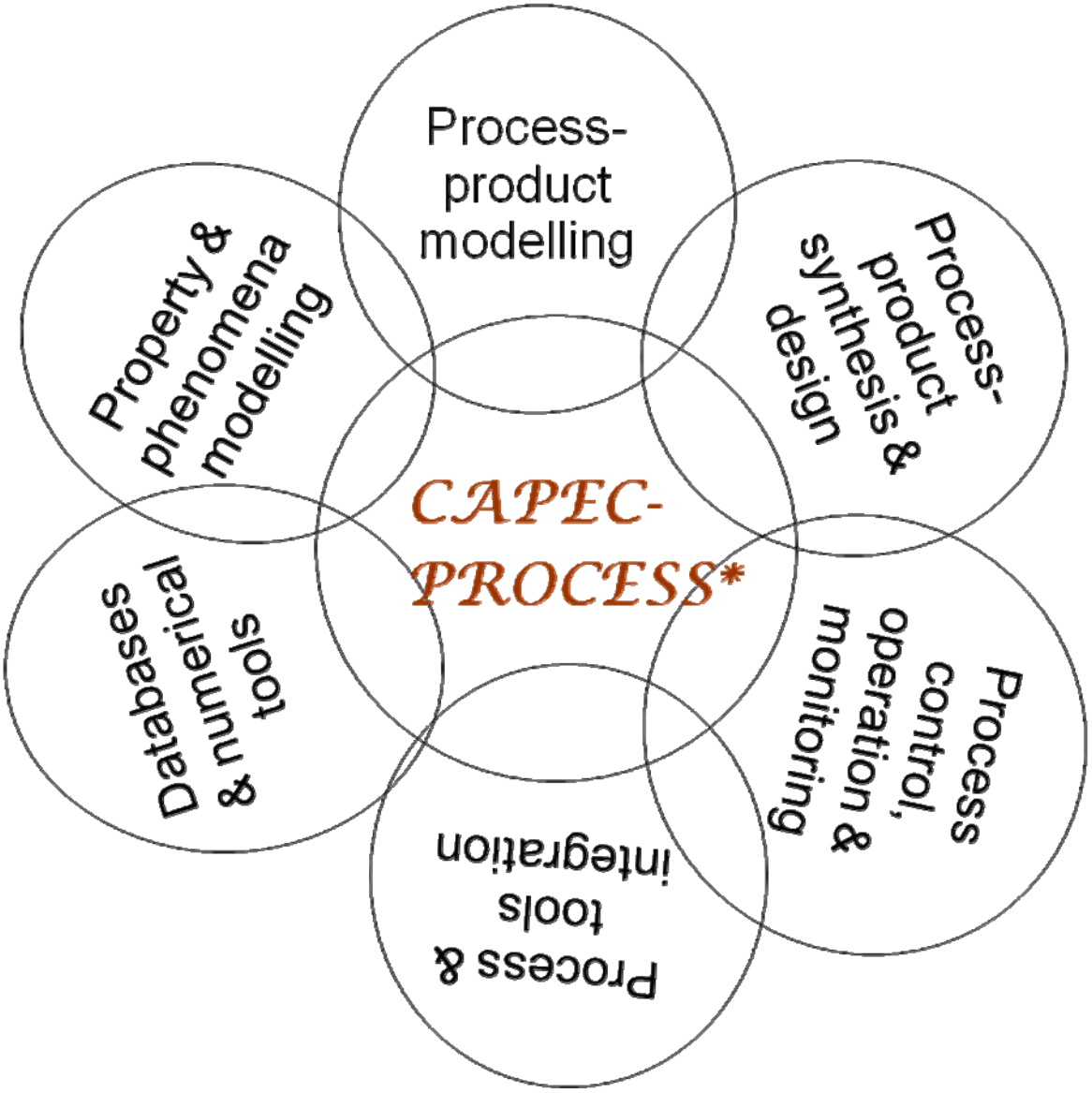
	G – Invited Seminars (from 2009)

G	Rafiqul Gani, 2009, “Multiscale and multidimension models for process product design”, Chemical Engineering, TU-Dortmund, Germany, 3-4 February
G	Rafiqul Gani, 2009, “CAPEC and ICAS: Overview”, Cognis GmbH, Düsseldorf, Germany, 9 July
G	Rafiqul Gani, 2009, “Computer aided polymer design using multiscale modelling”, The Petroleum and Petrochemical College (PPC), Chulalongkorn University, Bangkok, Thailand, 5 October
G	Rafiqul Gani, 2009, “A process systems engineering approach for managing the complexity in product-process design”, PROSPECT, Universiti Teknologi Malaysia (UTM), Malaysia, 13-14 October
G	Rafiqul Gani, 2009, “Property modeling for applications in chemical product and process design”, National Institute of Standards and Technology (NIST), Boulder, CO, USA, 6 November
G	Gürkan Sin, 2009, “Reliability of Cellulose Hydrolysis Models to Support Biofuel Process Design - Identifiability and Uncertainty Analysis”, DuPont Engineering Research and Technology, Wilmington, Delaware, USA, 13 November
G	Rafiqul Gani, 2009, The Ginn Distinguished Lecture: “A Process Systems Engineering Approach for Managing the Complexity in Chemical Product-Process Design”, Auburn University, AL, USA, 16 November
G	Rafiqul Gani, 2009, “A Process Systems Engineering Approach for Managing the Complexity in Chemical Product-Process Design”, Department of Chemical Engineering, Virginia Polytechnic Institute and State University, USA, 18 November
G	Rafiqul Gani, 2009, “Solvent selection and design”, Green Chemistry Centre, York University, UK, 26-28 November
G	Rafiqul Gani, 2009, “A Process Systems Engineering Approach for Managing the Complexity in Chemical Product-Process Design”, Instituto Superior Tecnico, Dept. Engenharia Quimica e Biologica, Lisbon, Portugal, 11 December
	G – Invited Seminars 2010
G	Rafiqul Gani, 2010, “Solvent Selection and Design”, RWTH Aachen, Germany, 22 January
G	R. Gani, 2010, “Solvents, green chemistry and sustainable product-process design”, TU-Delft, TU-Eindhoven, University of Twente, The Netherlands, 7-9 April
G	R. Gani, 2010, “A process systems engineering approach to managing the complexity in chemical product process design”, Tsinghua University; Beijing, China, 14 May

	Accepted/planned conference presentations between June – December 2010
F	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, John Bagterp Jørgensen, **2010**, ”ARX-Model based Model Predictive Control with Offset-Free Tracking”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Ricardo Morales-Rodriguez, Marie Capron, Jakob Kjøbsted Huusom and Gürkan Sin, **2010**, ”Controlled fed-batch operation for enzymatic cellulose hydrolysis in 2G bioethanol production”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Oscar Andres Prado-Rubio, Sten Bay Jørgensen and Gunnar Jonsson, **2010**, ”Control System Development for Integrated Bioreactor and Membrane Separation Process”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Oscar Andres Prado-Rubio, John Bagterp Jørgensen and Sten Bay Jørgensen, **2010**, ”Systematic Model Analysis for Single Cell Protein (SCP) Production in a U-Loop Reactor”, ESCAPE20, Ischia, Naples, Italy, 6-9 June

F	Merlin Alvarado-Morales, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, **2010**, "Synthesis, Design and Analysis of Downstream Separation in Bio-refinery Processes through a Group-Contribution Approach", ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Alicia Román-Martinez, Philip Lutze, John M. Woodley, Rafiqul Gani, **2010**, "A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes", ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani, **2010**, "A computer-aided framework for regression and multi-scale-modelling needs in innovative product-process engineering", ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Elisa Conte, Rafiqul Gani, Tom Malik, **2010**, "The Virtual Product-Process Laboratory applied to personal care formulations", ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Noor Asma Fazli Abdul Samad, Ravendra Singh, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, **2010**, "Control of Process Operations and Monitoring of Product Qualities through Generic Model-based in Batch Cooling Crystallization", ESCAPE20, Ischia, Naples, Italy, 6-9 June
F	Singh, R., **2010**, "Model-based computer-aided framework for design of process monitoring and analysis systems (PAT systems)", Invited lecture, on the ceremony of EFCE Excellence Award for the Outstanding PhD Thesis on CAPE, from European Federation of Chemical Engineering (EFCE), ESCAPE 20, Ischia, Naples, Italy, 6-9 June **(Invited)**
F (poster)	Ricardo Morales-Rodriguez, Krist V. Gernaey, Anne S. Meyer, Gürkan Sin , **2010**, "Integrated Dynamic Plant-Wide Model-Based Simulation of Bioethanol Production from Lignocellulose", Dansk Kemiingeniørkonference – DK2-2010, 16-17 June, Lyngby, Denmark
F (poster)	Dres Foged Olsen, John Bagterp Jørgensen, John Villadsen, Sten Bay Jørgensen, **2010**, "Single-Cell Protein Production in a U-Loop Reactor", Dansk Kemiingeniørkonference - DK2-2010, 16-17 June, Lyngby, Denmark
F	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, **2010**, "Tuning of Methods for Offset Free MPC based on ARX Model Representations", American Control Conference (ACC), Baltimore, Maryland, USA, 30 June - 2 July
F	Dres Foged Olsen; John Bagterp Jørgensen; John Villadsen.; Sten Bay Jørgensen, **2010**, "Modeling and Simulation of Single Cell Protein Production", 11th Computer Applications in Biotechnology, CAB 2010, Leuven, Belgium, 5-7 July
F	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, **2010**, "Adaptive Disturbance Estimation for Offset-Free Model Predictive Control", 9th International Symposium on Dynamics and Control of Process Systems, DYCOPS, Leuven, Belgium, 7-9 July
F	Mohd. Kamaruddin Abd. Hamid, Gürkan Sin and Rafiqul Gani, **2010**, "Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problems for Reactor-Separator-Recycle Systems", 9th International Symposium on Dynamics and Control of Process Systems, DYCOPS, Leuven, Belgium, 7-9 July
F	Dres Foged Olsen; John Bagterp Jørgensen; John Villadsen.; Sten Bay Jørgensen, **2010**, " Optimal Operating Points for SCP Production in the U-Loop Reactor", 9th International Symposium on Dynamics and Control of Process Systems, DYCOPS 2010, Leuven, Belgium, 7-9 July
F	Singh, R., Gernaey, K. V., Gani, R., **2010**, "Systematic computer-aided method and tool (ICAS-PAT) for design, analysis &/or validation of process monitoring and analysis systems (PAT systems)", CHISA2010 - ECCE7 conference, Prague, Czech Republic, 28 August – 1 September

F	F. Muller, R. R. Sanchez, T. Wrate, S. Davison, A. Manipura, E. B. Martin, G. A. Montague, M. Kraut, K. Haas-Santo, K. Forsberg, A. C. Rasmuson, R. Singh, K. V. Gernaey, R. Gani, J. M. Woodley, **2010**, "F^3 process design for fine chemical and Pharmaceutical transformations", Oral presentation at CHISA2010 - ECCE7 conference, Prague, Czech Republic, 28 August – 1 September
F	R. Morales-Rodriguez, K.V. Gernaey, A.S. Meyer and G. Sin, 2010, "Dynamic plant-wide modelling for bioethanol production from lignocellulosic biomass (2G)", CHISA 2010, ECCE-7, Prague, Czech Republic, 29 August - 1 September
F (poster)	Samad, N. A. F. A., Singh, R., Sin, G., Gernaey, K. V., Gani, R., **2010**, "A Generic Model-Based Framework for Batch Cooling Crystallization Processes", PBM1010 (4th International Conference on Population Balance Modeling), Berlin, Germany, 15–17 September
F	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, **2010**, "Tuning of Offset-Free ARX-based SISO Model Predictive Control", 49th IEEE Conference on Decision and Control (CDC), CDC49, Atlanta, Georgia, USA, 15-17 December
F	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, **2010**, "Adaptive Disturbance Estimation for Offset-Free SISO Model Predictive Control", 49th IEEE Conference on Decision and Control (CDC), CDC49, Atlanta, Georgia, USA, 15-17 December



*** Systematic methods and tool**

Please contact Mrs. Eva Mikkelsen (eva@kt.dtu.dk) for further information